



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:46 AM UTC

PDB ID : 9T05 / pdb_00009t05
Title : X-ray structure of the adduct formed by dirhodium tetraacetate with a C-phycocyanin
Authors : Merlino, A.; Ferraro, G.
Deposited on : 2025-10-16
Resolution : 2.17 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

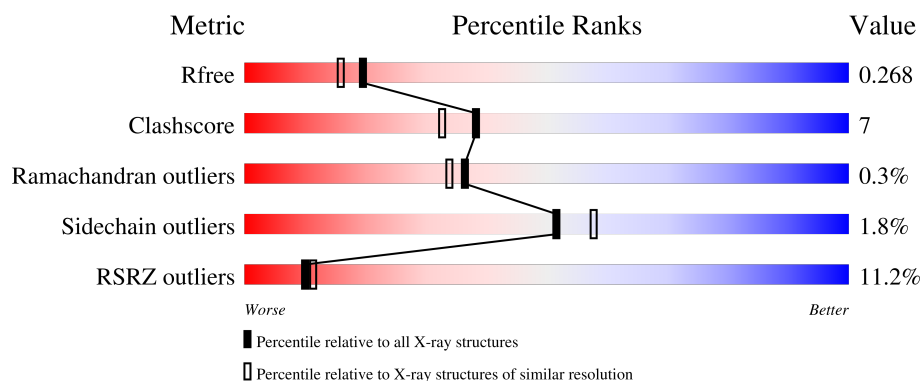
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.17 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AAA	162	12% 93% 6%
1	CCC	162	3% 94% 6%
1	EEE	162	8% 91% 8%
1	GGG	162	7% 94% 6%
1	III	162	4% 91% 8%

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Mol	Chain	Length	Quality of chain
1	KKK	162	14% 86% 13% .
2	BBB	173	20% 91% 9% .
2	DDD	173	9% 89% 10% ..
2	FFF	173	17% 87% 13% .
2	HHH	173	17% 93% 6% .
2	JJJ	173	11% 93% 6% .
2	LLL	173	9% 93% 6% ..

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 16492 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

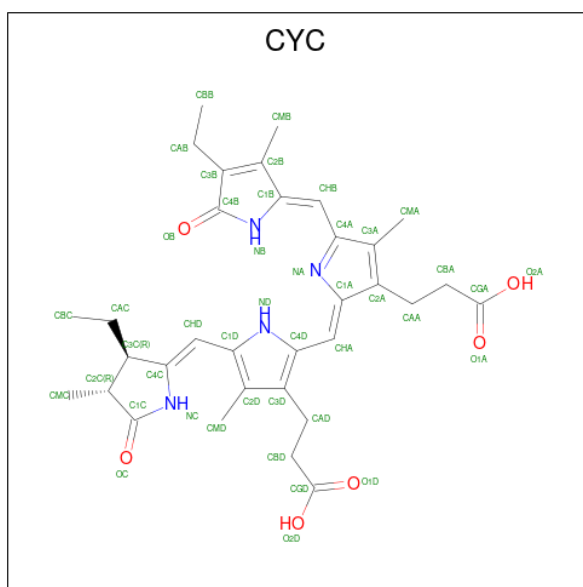
- Molecule 1 is a protein called C-phycocyanin alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	162	Total	C	N	O	S	0	3	0
			1240	771	217	244	8			
1	CCC	162	Total	C	N	O	S	0	2	0
			1221	760	210	243	8			
1	EEE	162	Total	C	N	O	S	0	3	0
			1237	769	217	243	8			
1	GGG	162	Total	C	N	O	S	0	5	0
			1241	770	214	249	8			
1	III	162	Total	C	N	O	S	0	4	0
			1243	772	218	245	8			
1	KKK	162	Total	C	N	O	S	0	4	0
			1247	775	216	248	8			

- Molecule 2 is a protein called C-phycocyanin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	BBB	172	Total	C	N	O	S	0	1	0
			1277	790	224	255	8			
2	DDD	172	Total	C	N	O	S	0	1	0
			1280	792	225	255	8			
2	FFF	172	Total	C	N	O	S	0	0	0
			1271	787	223	253	8			
2	HHH	172	Total	C	N	O	S	0	0	0
			1271	787	223	253	8			
2	JJJ	172	Total	C	N	O	S	0	2	0
			1291	798	228	257	8			
2	LLL	172	Total	C	N	O	S	0	0	0
			1271	787	223	253	8			

- Molecule 3 is PHYCOCYANOBILIN (CCD ID: CYC) (formula: $C_{33}H_{40}N_4O_6$).



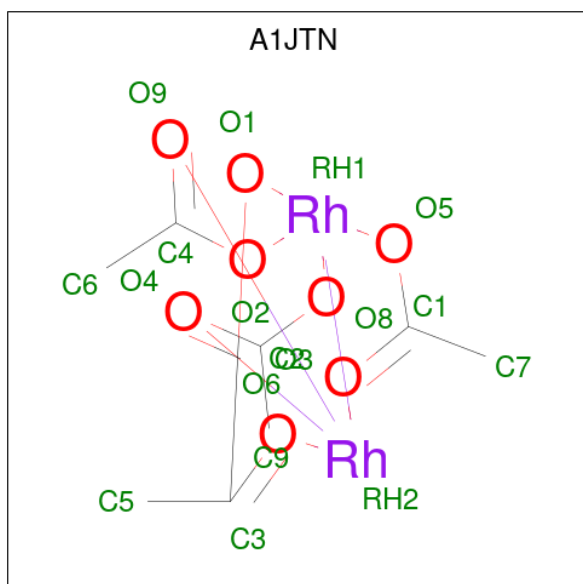
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	AAA	1	Total 43	C 33	N 4	O 6	0	0
3	BBB	1	Total 43	C 33	N 4	O 6	0	0
3	BBB	1	Total 43	C 33	N 4	O 6	0	0
3	CCC	1	Total 43	C 33	N 4	O 6	0	0
3	DDD	1	Total 43	C 33	N 4	O 6	0	0
3	DDD	1	Total 43	C 33	N 4	O 6	0	0
3	EEE	1	Total 43	C 33	N 4	O 6	0	0
3	FFF	1	Total 43	C 33	N 4	O 6	0	0
3	FFF	1	Total 43	C 33	N 4	O 6	0	0
3	GGG	1	Total 43	C 33	N 4	O 6	0	0
3	HHH	1	Total 43	C 33	N 4	O 6	0	0
3	HHH	1	Total 43	C 33	N 4	O 6	0	0
3	III	1	Total 43	C 33	N 4	O 6	0	0
3	JJJ	1	Total 43	C 33	N 4	O 6	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	JJJ	1	Total	C	N	O	0	0
			43	33	4	6		
3	KKK	1	Total	C	N	O	0	0
			43	33	4	6		
3	LLL	1	Total	C	N	O	0	0
			43	33	4	6		
3	LLL	1	Total	C	N	O	0	0
			43	33	4	6		

- Molecule 4 is dirhodium tetraacetate (CCD ID: A1JTN) (formula: $C_8H_{12}O_8Rh_2$) (labeled as "Ligand of Interest" by depositor).



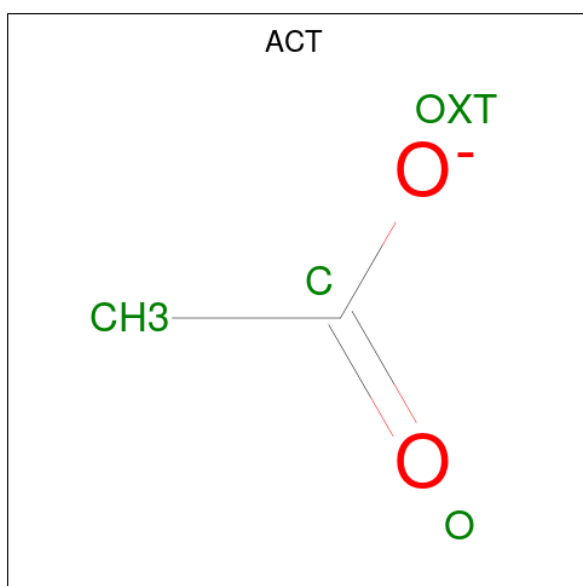
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	AAA	1	Total	Rh			0	0
			2	2				
4	BBB	1	Total	C	O	Rh	0	0
			18	8	8	2		
4	CCC	1	Total	Rh			0	0
			2	2				
4	DDD	1	Total	C	O	Rh	0	0
			18	8	8	2		
4	EEE	1	Total	Rh			0	0
			2	2				
4	FFF	1	Total	C	O	Rh	0	0
			18	8	8	2		
4	GGG	1	Total	Rh			0	0
			2	2				

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	HHH	1	Total C O Rh 18 8 8 2	0	0
4	III	1	Total Rh 2 2	0	0
4	JJJ	1	Total C O Rh 18 8 8 2	0	0
4	KKK	1	Total Rh 2 2	0	0
4	LLL	1	Total C O Rh 18 8 8 2	0	0

- Molecule 5 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	EEE	1	Total C O 4 2 2	0	0
5	FFF	1	Total C O 4 2 2	0	0
5	GGG	1	Total C O 4 2 2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	AAA	67	Total O 67 67	0	0

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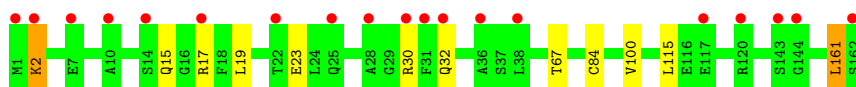
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	BBB	48	Total 48	O 48	0	0
6	CCC	68	Total 68	O 68	0	0
6	DDD	41	Total 41	O 41	0	0
6	EEE	49	Total 49	O 49	0	0
6	FFF	21	Total 21	O 21	0	0
6	GGG	37	Total 37	O 37	0	0
6	HHH	28	Total 28	O 28	0	0
6	III	44	Total 44	O 44	0	0
6	JJJ	17	Total 17	O 17	0	0
6	KKK	31	Total 32	O 32	0	1
6	LLL	44	Total 44	O 44	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

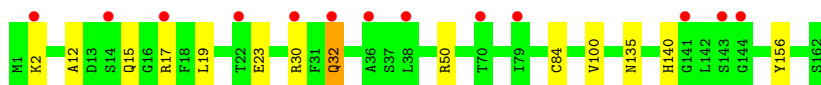
- Molecule 1: C-phycocyanin alpha subunit



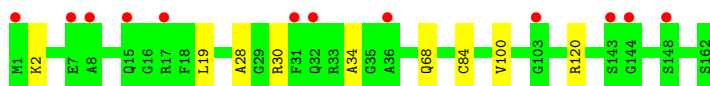
- Molecule 1: C-phycocyanin alpha subunit



- Molecule 1: C-phycocyanin alpha subunit



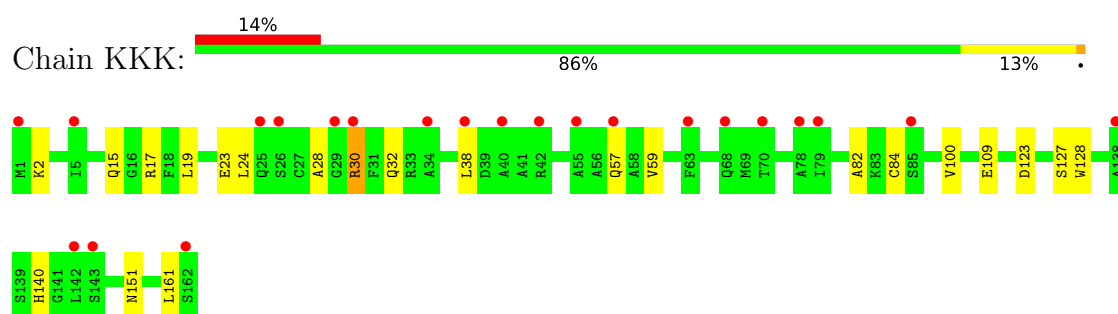
- Molecule 1: C-phycocyanin alpha subunit



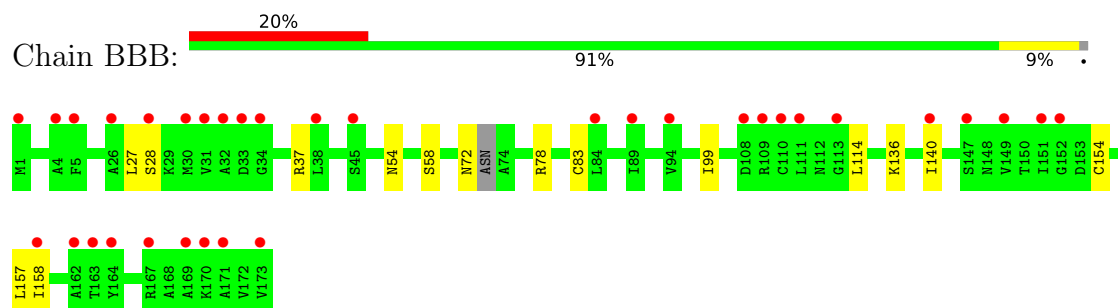
- Molecule 1: C-phycocyanin alpha subunit



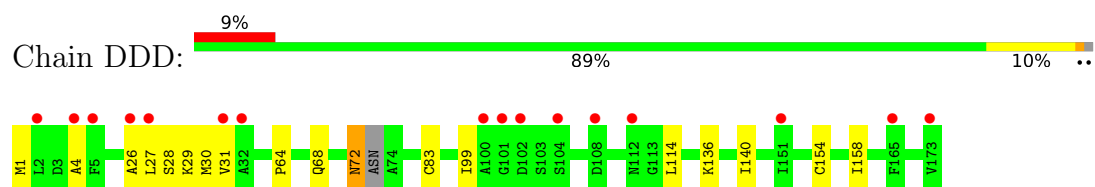
- Molecule 1: C-phycocyanin alpha subunit



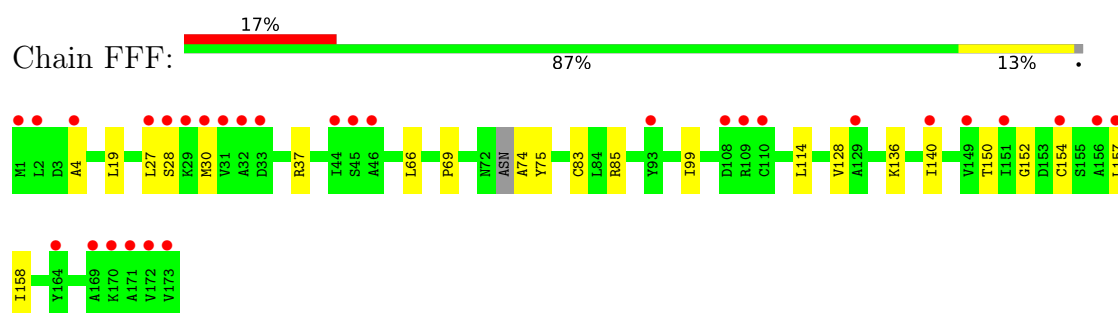
- Molecule 2: C-phycoerythrin beta chain



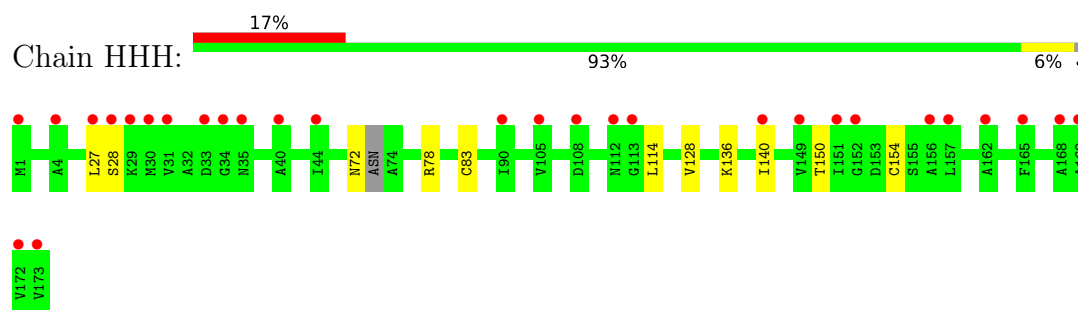
- Molecule 2: C-phycoerythrin beta chain



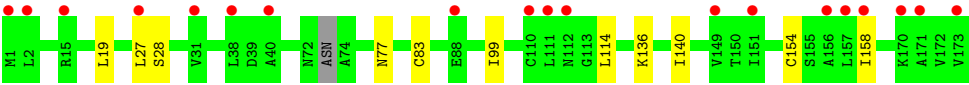
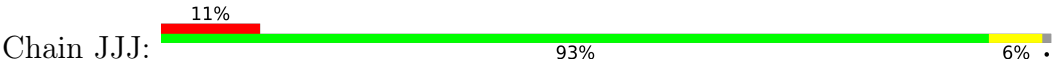
- Molecule 2: C-phycoerythrin beta chain



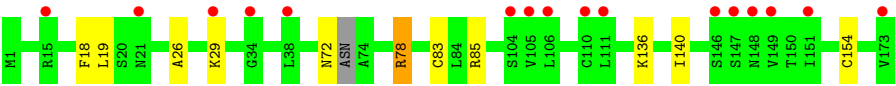
- Molecule 2: C-phycoerythrin beta chain



- Molecule 2: C-phycoerythrin beta chain



● Molecule 2: C-phycoyanin beta chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	60.59Å 188.50Å 207.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	139.83 – 2.17 139.44 – 2.17	Depositor EDS
% Data completeness (in resolution range)	81.2 (139.83-2.17) 81.2 (139.44-2.17)	Depositor EDS
R_{merge}	0.34	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.227 , 0.263 0.230 , 0.268	Depositor DCC
R_{free} test set	5000 reflections (3.95%)	wwPDB-VP
Wilson B-factor (Å ²)	31.9	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 20.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	16492	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.30% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MEN, ACT, DOD, CYC, A1JTN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	AAA	1.02	0/1261	1.53	0/1705
1	CCC	1.01	0/1242	1.53	4/1681 (0.2%)
1	EEE	1.03	0/1258	1.51	0/1702
1	GGG	1.05	0/1262	1.51	2/1708 (0.1%)
1	III	0.99	0/1264	1.51	1/1709 (0.1%)
1	KKK	1.01	0/1268	1.52	4/1715 (0.2%)
2	BBB	1.04	0/1279	1.54	0/1730
2	DDD	1.05	0/1282	1.54	0/1735
2	FFF	1.04	0/1273	1.53	0/1722
2	HHH	1.03	0/1273	1.54	0/1722
2	JJJ	1.03	0/1293	1.54	0/1748
2	LLL	1.04	0/1273	1.56	0/1722
All	All	1.03	0/15228	1.53	11/20599 (0.1%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	KKK	161	LEU	CA-C-N	7.81	135.77	121.70
1	KKK	161	LEU	C-N-CA	7.81	135.77	121.70
1	CCC	109	GLU	CB-CG-CD	7.38	125.15	112.60
1	III	39	ASP	CA-CB-CG	6.33	118.93	112.60
1	GGG	28	ALA	CA-C-N	5.68	126.39	120.03
1	GGG	28	ALA	C-N-CA	5.68	126.39	120.03
1	CCC	30	ARG	CG-CD-NE	-5.33	100.28	112.00
1	KKK	28	ALA	CA-C-N	5.22	125.88	120.03
1	KKK	28	ALA	C-N-CA	5.22	125.88	120.03
1	CCC	35	GLY	CA-C-N	5.13	127.11	120.44
1	CCC	35	GLY	C-N-CA	5.13	127.11	120.44

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AAA	1240	0	1215	24	0
1	CCC	1221	0	1193	9	0
1	EEE	1237	0	1215	23	0
1	GGG	1241	0	1207	13	0
1	III	1243	0	1218	14	0
1	KKK	1247	0	1215	20	0
2	BBB	1277	0	1281	21	0
2	DDD	1280	0	1284	22	0
2	FFF	1271	0	1276	28	0
2	HHH	1271	0	1277	21	0
2	JJJ	1291	0	1294	20	0
2	LLL	1271	0	1277	18	0
3	AAA	43	0	38	8	0
3	BBB	86	0	76	14	0
3	CCC	43	0	37	6	0
3	DDD	86	0	75	17	0
3	EEE	43	0	38	10	0
3	FFF	86	0	76	18	0
3	GGG	43	0	38	8	0
3	HHH	86	0	76	19	0
3	III	43	0	38	3	0
3	JJJ	86	0	76	14	0
3	KKK	43	0	38	6	0
3	LLL	86	0	76	15	0
4	AAA	2	0	0	0	0
4	BBB	18	0	0	0	0
4	CCC	2	0	0	0	0
4	DDD	18	0	0	1	0
4	EEE	2	0	0	0	0
4	FFF	18	0	0	0	0
4	GGG	2	0	0	0	0
4	HHH	18	0	0	0	0
4	III	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	JJJ	18	0	0	0	0
4	KKK	2	0	0	0	0
4	LLL	18	0	0	1	0
5	EEE	4	0	3	0	0
5	FFF	4	0	3	0	0
5	GGG	4	0	3	0	0
6	AAA	67	0	0	2	0
6	BBB	48	0	0	0	0
6	CCC	68	0	0	2	0
6	DDD	41	0	0	0	0
6	EEE	49	0	0	2	0
6	FFF	21	0	0	0	0
6	GGG	37	0	0	0	0
6	HHH	28	0	0	1	0
6	III	44	0	0	0	0
6	JJJ	17	0	0	0	0
6	KKK	32	0	0	2	0
6	LLL	44	0	0	0	0
All	All	16492	0	15643	218	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (218) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:GGG:84:CYS:SG	3:GGG:201:CYC:HAC2	1.22	1.71
1:III:84:CYS:SG	3:III:201:CYC:HAC2	1.15	1.70
2:FFF:154:CYS:SG	3:FFF:504:CYC:HAC1	1.28	1.69
2:HHH:154:CYS:SG	3:HHH:203:CYC:HAC1	1.24	1.69
1:AAA:84:CYS:SG	3:AAA:201:CYC:HAC2	1.13	1.68
2:DDD:154:CYS:SG	3:DDD:203:CYC:HAC1	1.20	1.67
2:HHH:83:CYS:SG	3:HHH:202:CYC:HAC2	1.25	1.67
2:FFF:83:CYS:SG	3:FFF:503:CYC:HAC2	1.33	1.66
1:KKK:84:CYS:SG	3:KKK:201:CYC:HAC2	1.30	1.65
2:LLL:83:CYS:SG	3:LLL:202:CYC:HAC2	1.38	1.62
2:BBB:83:CYS:SG	3:BBB:202:CYC:HAC2	1.40	1.62
2:BBB:154:CYS:SG	3:BBB:203:CYC:HAC1	1.39	1.60
2:LLL:154:CYS:SG	3:LLL:203:CYC:HAC1	1.42	1.58
2:JJJ:83:CYS:SG	3:JJJ:202:CYC:HAC2	1.44	1.52
1:CCC:84:CYS:SG	3:CCC:201:CYC:CAC	2.02	1.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:DDD:83:CYS:SG	3:DDD:202:CYC:CAC	2.06	1.44
1:AAA:84:CYS:SG	3:AAA:201:CYC:CAC	2.07	1.41
2:DDD:154:CYS:SG	3:DDD:203:CYC:CAC	2.08	1.40
2:JJJ:154:CYS:SG	3:JJJ:203:CYC:HAC1	1.59	1.40
1:III:84:CYS:SG	3:III:201:CYC:CAC	2.08	1.39
2:LLL:154:CYS:SG	3:LLL:203:CYC:CAC	2.09	1.39
2:HHH:83:CYS:SG	3:HHH:202:CYC:CAC	2.09	1.38
2:FFF:154:CYS:SG	3:FFF:504:CYC:CAC	2.12	1.36
1:EEE:84:CYS:SG	3:EEE:201:CYC:HAC2	1.64	1.36
1:GGG:84:CYS:SG	3:GGG:201:CYC:CAC	2.17	1.32
2:BBB:83:CYS:SG	3:BBB:202:CYC:CAC	2.20	1.30
2:FFF:83:CYS:SG	3:FFF:503:CYC:CAC	2.20	1.29
2:HHH:154:CYS:SG	3:HHH:203:CYC:CAC	2.20	1.28
2:LLL:83:CYS:SG	3:LLL:202:CYC:CAC	2.24	1.26
2:JJJ:154:CYS:SG	3:JJJ:203:CYC:CAC	2.23	1.24
2:JJJ:83:CYS:SG	3:JJJ:202:CYC:CAC	2.25	1.24
2:BBB:154:CYS:SG	3:BBB:203:CYC:CAC	2.27	1.21
1:KKK:84:CYS:SG	3:KKK:201:CYC:CAC	2.26	1.21
1:EEE:84:CYS:SG	3:EEE:201:CYC:CAC	2.30	1.19
2:DDD:154:CYS:HG	3:DDD:203:CYC:HAC1	1.18	0.99
1:EEE:84:CYS:SG	3:EEE:201:CYC:CBC	2.53	0.97
2:LLL:154:CYS:SG	3:LLL:203:CYC:HAC2	2.05	0.94
2:FFF:154:CYS:HG	3:FFF:504:CYC:HAC1	1.09	0.91
2:HHH:83:CYS:SG	3:HHH:202:CYC:CBC	2.59	0.90
2:BBB:83:CYS:SG	3:BBB:202:CYC:CBC	2.61	0.87
2:JJJ:154:CYS:SG	3:JJJ:203:CYC:HAC2	2.17	0.84
1:EEE:84:CYS:SG	3:EEE:201:CYC:HBC2	2.18	0.83
2:DDD:83:CYS:SG	3:DDD:202:CYC:CBC	2.68	0.82
1:CCC:84:CYS:SG	3:CCC:201:CYC:CBC	2.68	0.80
1:EEE:15:GLN:HE21	1:EEE:17[B]:ARG:HD3	1.46	0.80
2:JJJ:83:CYS:SG	3:JJJ:202:CYC:CBC	2.70	0.80
1:AAA:115:LEU:HD21	1:AAA:161:LEU:HD13	1.66	0.78
1:III:100:VAL:HG21	2:LLL:19:LEU:HD12	1.68	0.75
2:FFF:83:CYS:SG	3:FFF:503:CYC:CBC	2.75	0.75
2:FFF:154:CYS:SG	3:FFF:504:CYC:HAC2	2.27	0.74
1:AAA:84:CYS:SG	3:AAA:201:CYC:CBC	2.76	0.73
1:AAA:84:CYS:CB	3:AAA:201:CYC:HAC2	2.17	0.72
2:LLL:154:CYS:HG	3:LLL:203:CYC:HAC1	0.90	0.72
2:HHH:83:CYS:CB	3:HHH:202:CYC:HAC2	2.20	0.72
1:CCC:149:GLU:OE1	6:CCC:301:HOH:O	2.08	0.71
2:LLL:83:CYS:SG	3:LLL:202:CYC:CBC	2.78	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:DDD:99:ILE:HG21	1:GGG:19:LEU:HD11	1.74	0.70
2:HHH:150:THR:OG1	3:HHH:203:CYC:O1A	2.11	0.69
2:BBB:83:CYS:CB	3:BBB:202:CYC:HAC2	2.23	0.68
2:BBB:154:CYS:CB	3:BBB:203:CYC:HAC1	2.24	0.68
2:JJJ:27:LEU:HD13	1:KKK:100:VAL:HG13	1.76	0.68
2:DDD:154:CYS:SG	3:DDD:203:CYC:C3C	2.82	0.67
1:III:100:VAL:HG21	2:LLL:19:LEU:CD1	2.24	0.67
1:KKK:140:HIS:HE1	1:KKK:151:ASN:OD1	1.78	0.66
2:DDD:72:MEN:HE22	3:DDD:202:CYC:HBD2	1.76	0.66
2:FFF:114:LEU:HD13	3:FFF:503:CYC:HMB3	1.77	0.65
1:CCC:30:ARG:HD2	1:CCC:30:ARG:O	1.97	0.65
1:AAA:115:LEU:HD21	1:AAA:161:LEU:CD1	2.27	0.65
1:III:15:GLN:HE21	1:III:17[A]:ARG:HD3	1.62	0.64
2:LLL:83:CYS:CB	3:LLL:202:CYC:HAC2	2.26	0.63
1:EEE:135:ASN:ND2	6:EEE:301:HOH:O	2.30	0.62
1:III:17[A]:ARG:NH2	1:III:23:GLU:OE1	2.32	0.62
1:AAA:100:VAL:HG13	2:FFF:27:LEU:HD13	1.81	0.61
1:EEE:84:CYS:SG	3:EEE:201:CYC:H2C	2.40	0.61
1:III:84:CYS:SG	3:III:201:CYC:CBC	2.88	0.61
2:BBB:54:ASN:O	2:BBB:58[B]:SER:OG	2.18	0.61
2:DDD:64:PRO:O	2:DDD:68[B]:GLN:HG2	2.02	0.60
2:DDD:27:LEU:HD13	1:GGG:100:VAL:HG13	1.84	0.59
3:BBB:203:CYC:HHD	3:BBB:203:CYC:HBC3	1.84	0.59
1:KKK:30[B]:ARG:HD3	1:KKK:30[B]:ARG:C	2.29	0.58
3:LLL:203:CYC:NB	3:LLL:203:CYC:HMA1	2.19	0.57
2:LLL:154:CYS:SG	3:LLL:203:CYC:C3C	2.90	0.57
2:LLL:154:CYS:HG	3:LLL:203:CYC:CAC	1.84	0.57
1:EEE:84:CYS:CB	3:EEE:201:CYC:HAC2	2.35	0.57
1:GGG:84:CYS:SG	3:GGG:201:CYC:CBC	2.92	0.57
1:AAA:67:THR:HG22	6:AAA:313:HOH:O	2.04	0.57
2:DDD:99:ILE:HG21	1:GGG:19:LEU:CD1	2.33	0.56
2:JJJ:83:CYS:CB	3:JJJ:202:CYC:HAC2	2.32	0.56
3:JJJ:203:CYC:NB	3:JJJ:203:CYC:HMA1	2.21	0.56
2:BBB:154:CYS:SG	3:BBB:203:CYC:CBC	2.94	0.55
2:DDD:83:CYS:SG	3:DDD:202:CYC:C3C	2.90	0.55
3:FFF:504:CYC:HMD1	3:FFF:504:CYC:HBD2	1.87	0.55
1:KKK:82:ALA:HB3	6:KKK:317:HOH:O	2.05	0.55
2:HHH:72:MEN:HE22	3:HHH:202:CYC:HBD2	1.87	0.55
2:FFF:83:CYS:CB	3:FFF:503:CYC:HAC2	2.30	0.55
2:JJJ:99:ILE:HG21	1:KKK:19:LEU:HD11	1.89	0.55
2:BBB:83:CYS:SG	3:BBB:202:CYC:HBC2	2.44	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BBB:27:LEU:HD13	1:EEE:100:VAL:HG13	1.87	0.55
2:BBB:154:CYS:SG	3:BBB:203:CYC:C3C	2.95	0.54
1:CCC:100:VAL:HG13	2:HHH:27:LEU:HD13	1.90	0.54
1:III:2:LYS:NZ	1:KKK:23:GLU:OE2	2.40	0.54
3:HHH:203:CYC:HBC3	3:HHH:203:CYC:HHD	1.89	0.54
2:BBB:99:ILE:HG21	1:EEE:19:LEU:HD11	1.90	0.54
2:HHH:154:CYS:SG	3:HHH:203:CYC:C3C	2.93	0.54
2:FFF:114:LEU:CD1	3:FFF:503:CYC:HMB3	2.37	0.54
1:III:12:ALA:HA	1:III:17[A]:ARG:NH1	2.23	0.53
1:EEE:15:GLN:NE2	1:EEE:17[B]:ARG:HD3	2.22	0.53
2:JJJ:114:LEU:CD1	3:JJJ:202:CYC:HMB3	2.39	0.53
2:BBB:114:LEU:HD13	3:BBB:202:CYC:HMB3	1.90	0.52
2:JJJ:114:LEU:HD13	3:JJJ:202:CYC:HMB3	1.91	0.52
2:JJJ:154:CYS:SG	3:JJJ:203:CYC:C3C	2.95	0.52
2:HHH:83:CYS:SG	3:HHH:202:CYC:HBC2	2.48	0.52
2:FFF:85:ARG:NH1	3:FFF:503:CYC:O1A	2.40	0.52
2:HHH:83:CYS:SG	3:HHH:202:CYC:C3C	2.93	0.52
3:DDD:202:CYC:HMA2	3:DDD:202:CYC:HB	1.75	0.52
1:AAA:32:GLN:NE2	1:EEE:32:GLN:HE21	2.08	0.51
1:GGG:84:CYS:HA	3:GGG:201:CYC:HHD	1.91	0.51
1:AAA:84:CYS:HA	3:AAA:201:CYC:HHD	1.93	0.51
3:DDD:202:CYC:HB	3:DDD:202:CYC:CMA	2.23	0.51
2:FFF:83:CYS:SG	3:FFF:503:CYC:C3C	2.98	0.50
2:JJJ:27:LEU:CD1	1:KKK:100:VAL:HG13	2.42	0.50
2:JJJ:83:CYS:SG	3:JJJ:202:CYC:HBC2	2.50	0.50
2:BBB:114:LEU:CD1	3:BBB:202:CYC:HMB3	2.41	0.50
2:BBB:78:ARG:HD3	6:CCC:320:HOH:O	2.11	0.50
2:FFF:150:THR:OG1	3:FFF:504:CYC:O1A	2.24	0.50
2:DDD:26:ALA:HB1	4:DDD:201:A1JTN:C2	2.41	0.49
1:III:15:GLN:NE2	1:III:17[A]:ARG:HH11	2.10	0.49
1:KKK:140:HIS:CE1	1:KKK:151:ASN:OD1	2.64	0.49
2:LLL:85:ARG:NH1	3:LLL:202:CYC:O1A	2.37	0.49
1:AAA:17[B]:ARG:NH2	6:AAA:305:HOH:O	2.44	0.49
1:AAA:84:CYS:SG	3:AAA:201:CYC:H2C	2.53	0.48
2:HHH:150:THR:HG1	3:HHH:203:CYC:CGA	2.22	0.48
1:AAA:84:CYS:SG	3:AAA:201:CYC:C3C	2.97	0.48
1:EEE:84:CYS:SG	3:EEE:201:CYC:C3C	3.01	0.48
2:DDD:27:LEU:CD1	1:GGG:100:VAL:HG13	2.43	0.48
3:EEE:201:CYC:HBC2	3:EEE:201:CYC:HMC1	1.94	0.48
2:BBB:37:ARG:HA	2:BBB:157:LEU:HD21	1.94	0.48
1:EEE:12:ALA:HA	1:EEE:17[B]:ARG:NH1	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:FFF:154:CYS:HG	3:FFF:504:CYC:CAC	1.99	0.48
2:HHH:83:CYS:HA	3:HHH:202:CYC:HHD	1.95	0.48
1:EEE:84:CYS:SG	3:EEE:201:CYC:C2C	3.02	0.47
2:BBB:99:ILE:HG21	1:EEE:19:LEU:CD1	2.44	0.47
2:FFF:154:CYS:SG	3:FFF:504:CYC:C3C	2.98	0.47
2:BBB:27:LEU:CD1	1:EEE:100:VAL:HG13	2.44	0.47
1:GGG:120:ARG:HD3	1:III:116:GLU:HG2	1.97	0.47
2:DDD:114:LEU:HD13	3:DDD:202:CYC:HMB3	1.97	0.47
1:AAA:100:VAL:HG13	2:FFF:27:LEU:CD1	2.44	0.46
2:JJJ:99:ILE:HG21	1:KKK:19:LEU:CD1	2.46	0.46
1:AAA:15:GLN:HE21	1:AAA:17[B]:ARG:HD3	1.80	0.46
3:DDD:203:CYC:HMD2	3:DDD:203:CYC:HC	1.80	0.46
2:JJJ:83:CYS:SG	3:JJJ:202:CYC:C3C	3.02	0.46
1:KKK:30[B]:ARG:HD3	1:KKK:30[B]:ARG:O	2.16	0.46
2:LLL:78:ARG:NH2	3:LLL:202:CYC:O2D	2.44	0.46
2:HHH:78:ARG:NH1	6:HHH:302:HOH:O	2.47	0.45
1:CCC:84:CYS:SG	3:CCC:201:CYC:C3C	2.97	0.45
2:FFF:140:ILE:HD12	2:FFF:158:ILE:HG23	1.96	0.45
2:DDD:83:CYS:SG	3:DDD:202:CYC:H2C	2.56	0.45
2:HHH:136:LYS:O	2:HHH:140:ILE:HG13	2.17	0.45
1:III:2:LYS:CE	1:KKK:15:GLN:HE22	2.30	0.45
1:EEE:140:HIS:CE1	6:EEE:326:HOH:O	2.70	0.45
2:JJJ:136:LYS:O	2:JJJ:140:ILE:HG12	2.17	0.44
2:FFF:136:LYS:O	2:FFF:140:ILE:HG12	2.17	0.44
1:EEE:15:GLN:HE21	1:EEE:17[A]:ARG:HD3	1.82	0.44
2:FFF:128:VAL:HG22	3:FFF:503:CYC:H3C	2.00	0.44
2:JJJ:140:ILE:HD12	2:JJJ:158:ILE:HG23	2.00	0.44
1:CCC:84:CYS:SG	3:CCC:201:CYC:H2C	2.58	0.44
3:CCC:201:CYC:HMC1	3:CCC:201:CYC:HBC2	1.99	0.44
2:FFF:4:ALA:HB3	2:FFF:30:MET:HE3	2.00	0.44
2:HHH:114:LEU:CD1	3:HHH:202:CYC:HMB3	2.48	0.44
1:KKK:84:CYS:SG	3:KKK:201:CYC:H2C	2.58	0.44
2:DDD:136:LYS:O	2:DDD:140:ILE:HG12	2.18	0.44
1:AAA:17[B]:ARG:NH1	1:AAA:23:GLU:OE1	2.48	0.44
1:AAA:19:LEU:HD11	2:FFF:99:ILE:HG21	2.00	0.44
1:AAA:19:LEU:CD1	2:FFF:99:ILE:HG21	2.48	0.43
2:FFF:66:LEU:O	2:FFF:74:ALA:HB3	2.18	0.43
2:DDD:140:ILE:HD12	2:DDD:158:ILE:HG23	2.00	0.43
1:KKK:38:LEU:HB2	6:KKK:304:HOH:O	2.18	0.43
2:LLL:83:CYS:SG	3:LLL:202:CYC:C3C	3.04	0.43
2:HHH:114:LEU:HD13	3:HHH:202:CYC:HMB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:III:45:THR:HG23	2:LLL:18:PHE:HB3	1.99	0.43
2:LLL:136:LYS:O	2:LLL:140:ILE:HG12	2.18	0.43
2:BBB:136:LYS:O	2:BBB:140:ILE:HG12	2.17	0.43
3:JJJ:202:CYC:HC	3:JJJ:202:CYC:CMD	2.31	0.43
1:KKK:128:TRP:CD2	3:KKK:201:CYC:HMC3	2.54	0.43
1:AAA:100:VAL:HG21	2:FFF:19:LEU:HD22	1.99	0.43
2:BBB:140:ILE:HD12	2:BBB:158:ILE:HG23	2.00	0.43
1:AAA:15:GLN:HE21	1:AAA:17[A]:ARG:HD3	1.83	0.43
3:DDD:202:CYC:CMD	3:DDD:202:CYC:HC	2.32	0.42
1:EEE:84:CYS:HA	3:EEE:201:CYC:HHD	2.00	0.42
1:GGG:84:CYS:SG	3:GGG:201:CYC:H2C	2.59	0.42
1:CCC:84:CYS:CB	3:CCC:201:CYC:CAC	2.94	0.42
3:DDD:203:CYC:HC	3:DDD:203:CYC:CMD	2.32	0.42
1:KKK:15:GLN:HE21	1:KKK:17:ARG:HD3	1.83	0.42
1:AAA:32:GLN:NE2	1:EEE:32:GLN:NE2	2.68	0.42
2:DDD:114:LEU:CD1	3:DDD:202:CYC:HMB3	2.49	0.42
1:GGG:84:CYS:CB	3:GGG:201:CYC:HAC2	2.33	0.42
1:KKK:59:VAL:HG11	3:KKK:201:CYC:HMC1	2.01	0.42
2:HHH:128:VAL:HG22	3:HHH:202:CYC:H3C	2.02	0.42
2:DDD:154:CYS:SG	3:DDD:203:CYC:HAC2	2.37	0.42
2:HHH:83:CYS:HA	3:HHH:202:CYC:CHD	2.49	0.42
2:LLL:26:ALA:HB1	4:LLL:201:A1JTN:C4	2.51	0.41
2:JJJ:77:ASN:HD22	2:JJJ:77:ASN:HA	1.73	0.41
1:AAA:2:LYS:NZ	1:EEE:23:GLU:OE2	2.53	0.41
1:AAA:84:CYS:SG	3:AAA:201:CYC:C2C	3.09	0.41
3:BBB:203:CYC:HB	3:BBB:203:CYC:CMA	2.34	0.41
1:GGG:84:CYS:SG	3:GGG:201:CYC:C3C	3.01	0.41
2:JJJ:19:LEU:HD22	1:KKK:100:VAL:HG21	2.02	0.41
2:HHH:154:CYS:SG	3:HHH:203:CYC:CBC	3.04	0.41
1:III:24:LEU:HB3	3:LLL:203:CYC:HBB3	2.03	0.41
1:AAA:17[A]:ARG:NH1	1:EEE:156:TYR:OH	2.53	0.41
2:DDD:4:ALA:HB3	2:DDD:30:MET:HE3	2.03	0.41
2:DDD:31:VAL:HG11	1:GGG:34:ALA:HB3	2.03	0.41
2:FFF:37:ARG:HA	2:FFF:157:LEU:HD21	2.02	0.41
1:KKK:84:CYS:HA	3:KKK:201:CYC:HHD	2.03	0.41
2:FFF:152:GLY:N	3:FFF:504:CYC:OC	2.54	0.40
2:FFF:69:PRO:HA	2:FFF:75:TYR:CG	2.56	0.40
3:GGG:201:CYC:HHA	3:GGG:201:CYC:HBD1	2.03	0.40
1:CCC:1:MET:HE1	1:CCC:110:TYR:OH	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AAA	163/162 (101%)	159 (98%)	3 (2%)	1 (1%)	21	15
1	CCC	162/162 (100%)	158 (98%)	3 (2%)	1 (1%)	21	15
1	EEE	163/162 (101%)	159 (98%)	3 (2%)	1 (1%)	21	15
1	GGG	165/162 (102%)	161 (98%)	3 (2%)	1 (1%)	21	15
1	III	164/162 (101%)	160 (98%)	3 (2%)	1 (1%)	21	15
1	KKK	164/162 (101%)	160 (98%)	3 (2%)	1 (1%)	21	15
2	BBB	170/173 (98%)	167 (98%)	3 (2%)	0	100	100
2	DDD	170/173 (98%)	167 (98%)	3 (2%)	0	100	100
2	FFF	169/173 (98%)	166 (98%)	3 (2%)	0	100	100
2	HHH	169/173 (98%)	166 (98%)	3 (2%)	0	100	100
2	JJJ	171/173 (99%)	168 (98%)	3 (2%)	0	100	100
2	LLL	169/173 (98%)	166 (98%)	3 (2%)	0	100	100
All	All	1999/2010 (100%)	1957 (98%)	36 (2%)	6 (0%)	36	34

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	III	2	LYS
1	KKK	2	LYS
1	AAA	2	LYS
1	CCC	2	LYS
1	EEE	2	LYS
1	GGG	2	LYS

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar

resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AAA	126/123 (102%)	123 (98%)	3 (2%)	43	47
1	CCC	125/123 (102%)	124 (99%)	1 (1%)	73	79
1	EEE	126/123 (102%)	122 (97%)	4 (3%)	34	36
1	GGG	128/123 (104%)	126 (98%)	2 (2%)	55	61
1	III	127/123 (103%)	123 (97%)	4 (3%)	35	37
1	KKK	127/123 (103%)	118 (93%)	9 (7%)	13	8
2	BBB	131/131 (100%)	130 (99%)	1 (1%)	73	79
2	DDD	131/131 (100%)	128 (98%)	3 (2%)	44	49
2	FFF	130/131 (99%)	129 (99%)	1 (1%)	73	79
2	HHH	130/131 (99%)	129 (99%)	1 (1%)	73	79
2	JJJ	132/131 (101%)	131 (99%)	1 (1%)	73	79
2	LLL	130/131 (99%)	128 (98%)	2 (2%)	57	64
All	All	1543/1524 (101%)	1511 (98%)	32 (2%)	51	52

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	30[A]	ARG
1	AAA	30[B]	ARG
1	AAA	161	LEU
2	BBB	28	SER
1	CCC	68	GLN
2	DDD	1	MET
2	DDD	28	SER
2	DDD	29	LYS
1	EEE	30[A]	ARG
1	EEE	30[B]	ARG
1	EEE	32	GLN
1	EEE	50	ARG
2	FFF	28	SER
1	GGG	30	ARG
1	GGG	68	GLN
2	HHH	28	SER
1	III	30[A]	ARG
1	III	30[B]	ARG

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Mol	Chain	Res	Type
1	III	57	GLN
1	III	68	GLN
2	JJJ	28	SER
1	KKK	24	LEU
1	KKK	30[A]	ARG
1	KKK	30[B]	ARG
1	KKK	32	GLN
1	KKK	57[A]	GLN
1	KKK	57[B]	GLN
1	KKK	109	GLU
1	KKK	123	ASP
1	KKK	127	SER
2	LLL	29	LYS
2	LLL	78	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

6 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	MEN	DDD	72	2	7,8,9	0.92	1 (14%)	4,9,11	0.60	0
2	MEN	LLL	72	2	7,8,9	0.84	1 (14%)	4,9,11	0.23	0
2	MEN	BBB	72	2	7,8,9	0.85	1 (14%)	4,9,11	0.91	0
2	MEN	HHH	72	2	7,8,9	0.71	0	4,9,11	0.30	0
2	MEN	FFF	72	2	7,8,9	0.71	0	4,9,11	0.33	0
2	MEN	JJJ	72	2	7,8,9	0.68	0	4,9,11	0.31	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MEN	DDD	72	2	-	2/7/8/10	-
2	MEN	LLL	72	2	-	5/7/8/10	-
2	MEN	BBB	72	2	-	2/7/8/10	-
2	MEN	HHH	72	2	-	3/7/8/10	-
2	MEN	FFF	72	2	-	2/7/8/10	-
2	MEN	JJJ	72	2	-	4/7/8/10	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	DDD	72	MEN	O-C	2.18	1.28	1.20
2	LLL	72	MEN	O-C	2.18	1.28	1.20
2	BBB	72	MEN	O-C	2.11	1.28	1.20

There are no bond angle outliers.

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	HHH	72	MEN	O-C-CA-CB
2	JJJ	72	MEN	CB-CG-ND2-CE2
2	LLL	72	MEN	O-C-CA-CB
2	LLL	72	MEN	CB-CG-ND2-CE2
2	JJJ	72	MEN	OD1-CG-ND2-CE2
2	LLL	72	MEN	OD1-CG-ND2-CE2
2	FFF	72	MEN	CA-CB-CG-OD1
2	DDD	72	MEN	CA-CB-CG-OD1
2	BBB	72	MEN	CA-CB-CG-OD1
2	JJJ	72	MEN	CA-CB-CG-OD1
2	BBB	72	MEN	CA-CB-CG-ND2
2	FFF	72	MEN	CA-CB-CG-ND2
2	HHH	72	MEN	CA-CB-CG-OD1
2	DDD	72	MEN	CA-CB-CG-ND2
2	HHH	72	MEN	CA-CB-CG-ND2
2	JJJ	72	MEN	CA-CB-CG-ND2
2	LLL	72	MEN	CA-CB-CG-ND2

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Mol	Chain	Res	Type	Atoms
2	LLL	72	MEN	CA-CB-CG-OD1

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	DDD	72	MEN	1	0
2	HHH	72	MEN	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

33 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	A1JTN	III	202	1	0,1,21	-	-	-		
3	CYC	KKK	201	-	46,46,46	1.00	1 (2%)	63,67,67	1.11	3 (4%)
4	A1JTN	EEE	203	1	0,1,21	-	-	-		
4	A1JTN	AAA	202	1	0,1,21	-	-	-		
3	CYC	JJJ	202	-	46,46,46	0.88	2 (4%)	63,67,67	1.15	4 (6%)
3	CYC	BBB	202	-	46,46,46	0.85	1 (2%)	63,67,67	1.31	8 (12%)
3	CYC	CCC	201	-	46,46,46	0.82	0	63,67,67	1.15	4 (6%)
3	CYC	GGG	201	-	46,46,46	1.05	3 (6%)	63,67,67	1.10	2 (3%)
3	CYC	BBB	203	-	46,46,46	0.95	1 (2%)	63,67,67	1.09	4 (6%)
4	A1JTN	HHH	201	2,6	4,21,21	1.43	1 (25%)	4,40,40	1.36	0
4	A1JTN	BBB	201	2,6	4,21,21	1.46	1 (25%)	4,40,40	1.75	1 (25%)
4	A1JTN	KKK	202	1	0,1,21	-	-	-		
5	ACT	FFF	501	-	3,3,3	1.41	0	3,3,3	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	A1JTN	JJJ	201	2,6	4,21,21	1.43	1 (25%)	4,40,40	1.55	1 (25%)
3	CYC	LLL	202	-	46,46,46	0.85	1 (2%)	63,67,67	1.10	4 (6%)
4	A1JTN	LLL	201	2,6	4,21,21	1.48	1 (25%)	4,40,40	1.84	1 (25%)
3	CYC	HHH	202	-	46,46,46	0.82	0	63,67,67	1.26	6 (9%)
3	CYC	HHH	203	-	46,46,46	0.80	1 (2%)	63,67,67	1.00	3 (4%)
4	A1JTN	GGG	203	1	0,1,21	-	-	-	-	-
3	CYC	DDD	202	-	46,46,46	1.01	4 (8%)	63,67,67	1.26	5 (7%)
4	A1JTN	CCC	202	1	0,1,21	-	-	-	-	-
3	CYC	JJJ	203	-	46,46,46	0.76	2 (4%)	63,67,67	1.11	3 (4%)
3	CYC	EEE	201	-	46,46,46	0.95	3 (6%)	63,67,67	1.03	3 (4%)
4	A1JTN	FFF	502	2,6	4,21,21	1.43	1 (25%)	4,40,40	1.38	1 (25%)
3	CYC	AAA	201	-	46,46,46	0.92	3 (6%)	63,67,67	1.08	1 (1%)
3	CYC	FFF	504	-	46,46,46	0.75	0	63,67,67	1.03	2 (3%)
3	CYC	DDD	203	-	46,46,46	0.88	2 (4%)	63,67,67	0.99	5 (7%)
3	CYC	III	201	-	46,46,46	1.23	3 (6%)	63,67,67	1.20	6 (9%)
4	A1JTN	DDD	201	2,6	4,21,21	1.49	1 (25%)	4,40,40	1.94	1 (25%)
3	CYC	FFF	503	-	46,46,46	0.79	0	63,67,67	1.31	5 (7%)
5	ACT	EEE	202	-	3,3,3	1.13	0	3,3,3	0.75	0
3	CYC	LLL	203	-	46,46,46	0.73	0	63,67,67	1.09	3 (4%)
5	ACT	GGG	202	-	3,3,3	1.03	0	3,3,3	1.39	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CYC	KKK	201	-	-	10/26/74/74	0/4/4/4
3	CYC	JJJ	202	-	-	8/26/74/74	0/4/4/4
3	CYC	BBB	202	-	-	12/26/74/74	0/4/4/4
3	CYC	CCC	201	-	-	7/26/74/74	0/4/4/4
3	CYC	GGG	201	-	-	11/26/74/74	0/4/4/4
3	CYC	BBB	203	-	-	9/26/74/74	0/4/4/4
4	A1JTN	HHH	201	2,6	-	-	0/4/4/4
4	A1JTN	BBB	201	2,6	-	-	0/4/4/4
4	A1JTN	JJJ	201	2,6	-	-	0/4/4/4
3	CYC	LLL	202	-	-	7/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	A1JTN	LLL	201	2,6	-	-	0/4/4/4
3	CYC	HHH	202	-	-	10/26/74/74	0/4/4/4
3	CYC	HHH	203	-	-	10/26/74/74	0/4/4/4
3	CYC	DDD	202	-	-	8/26/74/74	0/4/4/4
3	CYC	JJJ	203	-	-	12/26/74/74	0/4/4/4
3	CYC	EEE	201	-	-	10/26/74/74	0/4/4/4
4	A1JTN	FFF	502	2,6	-	-	0/4/4/4
3	CYC	AAA	201	-	-	9/26/74/74	0/4/4/4
3	CYC	FFF	504	-	-	16/26/74/74	0/4/4/4
3	CYC	DDD	203	-	-	9/26/74/74	0/4/4/4
3	CYC	III	201	-	-	9/26/74/74	0/4/4/4
4	A1JTN	DDD	201	2,6	-	-	0/4/4/4
3	CYC	FFF	503	-	-	10/26/74/74	0/4/4/4
3	CYC	LLL	203	-	-	13/26/74/74	0/4/4/4

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	III	201	CYC	CHD-C4C	4.49	1.43	1.36
3	KKK	201	CYC	CHD-C4C	3.39	1.42	1.36
3	GGG	201	CYC	CHD-C4C	3.36	1.42	1.36
3	III	201	CYC	C1B-C2B	-3.24	1.39	1.45
3	GGG	201	CYC	C1B-NB	3.16	1.43	1.37
3	EEE	201	CYC	C1B-C2B	-3.14	1.39	1.45
4	DDD	201	A1JTN	C7-C1	-2.91	1.37	1.49
4	LLL	201	A1JTN	C7-C1	-2.86	1.37	1.49
4	BBB	201	A1JTN	C7-C1	-2.85	1.37	1.49
4	FFF	502	A1JTN	C7-C1	-2.79	1.37	1.49
4	HHH	201	A1JTN	C7-C1	-2.79	1.37	1.49
4	JJJ	201	A1JTN	C7-C1	-2.78	1.37	1.49
3	DDD	202	CYC	CHD-C4C	2.72	1.41	1.36
3	GGG	201	CYC	CHD-C1D	2.60	1.46	1.40
3	BBB	203	CYC	CHD-C4C	2.54	1.40	1.36
3	DDD	203	CYC	CHD-C4C	2.41	1.40	1.36
3	EEE	201	CYC	CHD-C4C	2.40	1.40	1.36
3	JJJ	203	CYC	CHD-C4C	2.39	1.40	1.36
3	DDD	203	CYC	C1B-NB	2.39	1.41	1.37
3	JJJ	203	CYC	CHD-C1D	2.37	1.45	1.40
3	AAA	201	CYC	O2A-CGA	-2.32	1.23	1.30
3	EEE	201	CYC	O2A-CGA	-2.28	1.23	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	HHH	203	CYC	O2A-CGA	-2.13	1.23	1.30
3	DDD	202	CYC	C2C-C1C	-2.11	1.50	1.52
3	LLL	202	CYC	O2D-CGD	-2.10	1.23	1.30
3	III	201	CYC	OC-C1C	-2.10	1.19	1.23
3	JJJ	202	CYC	CHD-C4C	2.09	1.40	1.36
3	JJJ	202	CYC	CHD-C1D	2.08	1.45	1.40
3	BBB	202	CYC	C1B-C2B	-2.08	1.41	1.45
3	DDD	202	CYC	O2D-CGD	-2.07	1.24	1.30
3	AAA	201	CYC	C1B-C2B	-2.03	1.41	1.45
3	DDD	202	CYC	CHD-C1D	2.02	1.44	1.40
3	AAA	201	CYC	CHD-C1D	2.00	1.44	1.40

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	JJJ	203	CYC	CMB-C2B-C1B	4.87	130.08	124.16
3	FFF	503	CYC	CMB-C2B-C1B	4.40	129.51	124.16
3	BBB	203	CYC	CMB-C2B-C1B	4.35	129.45	124.16
3	HHH	202	CYC	CMB-C2B-C1B	4.25	129.33	124.16
3	CCC	201	CYC	CMB-C2B-C1B	4.11	129.16	124.16
3	DDD	202	CYC	CMB-C2B-C1B	3.91	128.91	124.16
3	BBB	202	CYC	CMB-C2B-C1B	3.80	128.78	124.16
3	KKK	201	CYC	CMB-C2B-C1B	3.63	128.57	124.16
3	HHH	203	CYC	CMB-C2B-C1B	3.57	128.50	124.16
3	BBB	202	CYC	CHD-C4C-NC	3.49	129.99	125.63
3	LLL	203	CYC	CMB-C2B-C1B	3.47	128.38	124.16
3	DDD	202	CYC	C1D-CHD-C4C	3.45	133.65	127.76
3	III	201	CYC	CAB-C3B-C2B	3.42	133.84	127.56
3	JJJ	202	CYC	CMB-C2B-C1B	3.41	128.31	124.16
4	DDD	201	A1JTN	O2-C4-C6	3.37	122.98	115.78
3	LLL	202	CYC	C1D-CHD-C4C	3.30	133.39	127.76
3	LLL	202	CYC	CMB-C2B-C1B	3.28	128.15	124.16
3	BBB	202	CYC	OC-C1C-C2C	-3.25	123.59	126.17
3	GGG	201	CYC	CMB-C2B-C1B	3.19	128.04	124.16
3	HHH	202	CYC	OC-C1C-C2C	-3.16	123.66	126.17
3	JJJ	202	CYC	C1D-CHD-C4C	3.13	133.11	127.76
3	FFF	503	CYC	C2C-C1C-NC	3.11	110.88	108.29
3	FFF	503	CYC	C1D-CHD-C4C	3.10	133.06	127.76
3	GGG	201	CYC	C3C-C4C-NC	-3.08	103.97	107.94
3	FFF	503	CYC	OC-C1C-C2C	-3.07	123.73	126.17
4	BBB	201	A1JTN	O2-C4-C6	3.06	122.33	115.78
3	FFF	504	CYC	CMB-C2B-C1B	3.04	127.85	124.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	BBB	202	CYC	C1D-CHD-C4C	3.02	132.92	127.76
3	HHH	202	CYC	C1D-CHD-C4C	2.92	132.74	127.76
3	HHH	203	CYC	CAC-C3C-C4C	2.83	119.94	112.67
3	EEE	201	CYC	CMB-C2B-C1B	2.77	127.53	124.16
3	BBB	202	CYC	C1B-NB-C4B	-2.71	107.34	110.66
3	DDD	202	CYC	C2C-C3C-C4C	2.71	105.39	101.34
4	JJJ	201	A1JTN	O2-C4-C6	2.69	121.53	115.78
3	FFF	503	CYC	C2C-C3C-C4C	2.59	105.21	101.34
3	CCC	201	CYC	CHB-C1B-C2B	-2.58	121.83	126.97
3	CCC	201	CYC	CAC-C3C-C4C	2.56	119.24	112.67
3	BBB	202	CYC	C2C-C3C-C4C	2.55	105.16	101.34
3	BBB	203	CYC	CAC-C3C-C4C	2.53	119.18	112.67
3	DDD	203	CYC	CMB-C2B-C1B	2.53	127.24	124.16
3	DDD	202	CYC	OC-C1C-C2C	-2.52	124.17	126.17
3	III	201	CYC	C3C-C4C-NC	-2.51	104.72	107.94
3	JJJ	202	CYC	C2C-C3C-C4C	2.50	105.09	101.34
3	III	201	CYC	CMA-C3A-C4A	2.47	128.93	125.10
3	JJJ	202	CYC	C1B-NB-C4B	-2.46	107.64	110.66
4	LLL	201	A1JTN	O2-C4-C6	2.45	121.02	115.78
3	LLL	203	CYC	C1B-CHB-C4A	2.44	134.04	128.06
3	JJJ	203	CYC	CMA-C3A-C4A	2.41	128.84	125.10
3	CCC	201	CYC	C1C-NC-C4C	-2.37	110.44	113.41
3	HHH	202	CYC	CHD-C4C-NC	2.34	128.55	125.63
3	LLL	202	CYC	C1B-NB-C4B	-2.33	107.80	110.66
3	HHH	202	CYC	C2C-C1C-NC	2.33	110.22	108.29
3	DDD	203	CYC	CHB-C1B-C2B	-2.30	122.38	126.97
3	FFF	504	CYC	CMA-C3A-C4A	2.25	128.59	125.10
3	III	201	CYC	CMB-C2B-C1B	2.23	126.87	124.16
3	HHH	202	CYC	C1C-NC-C4C	-2.22	110.63	113.41
3	DDD	202	CYC	CHD-C4C-NC	2.20	128.38	125.63
3	III	201	CYC	O1D-CGD-CBD	-2.19	116.15	123.09
3	KKK	201	CYC	O1A-CGA-CBA	-2.19	116.15	123.09
3	LLL	202	CYC	C1C-NC-C4C	-2.19	110.66	113.41
3	BBB	202	CYC	CAB-C3B-C2B	2.16	131.53	127.56
3	DDD	203	CYC	C2C-C3C-C4C	2.15	104.55	101.34
3	JJJ	203	CYC	O1A-CGA-CBA	-2.14	116.29	123.09
3	DDD	203	CYC	CHB-C1B-NB	2.13	130.61	126.06
3	III	201	CYC	O2D-CGD-CBD	2.10	120.64	114.00
3	EEE	201	CYC	C3C-C4C-NC	-2.09	105.25	107.94
3	BBB	203	CYC	CMA-C3A-C4A	2.09	128.35	125.10
3	LLL	203	CYC	CHB-C1B-C2B	-2.07	122.84	126.97
3	BBB	202	CYC	C2C-C1C-NC	2.07	110.01	108.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	BBB	203	CYC	C3B-C4B-NB	-2.07	105.12	106.77
4	FFF	502	A1JTN	O2-C4-C6	2.05	120.16	115.78
3	KKK	201	CYC	CAC-C3C-C4C	2.05	117.93	112.67
3	AAA	201	CYC	C1C-NC-C4C	-2.02	110.87	113.41
3	HHH	203	CYC	CHD-C4C-NC	-2.02	123.11	125.63
3	EEE	201	CYC	C1C-NC-C4C	-2.01	110.88	113.41
3	DDD	203	CYC	O1D-CGD-CBD	-2.00	116.73	123.09

There are no chirality outliers.

All (180) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	AAA	201	CYC	NA-C4A-CHB-C1B
3	AAA	201	CYC	C3A-C4A-CHB-C1B
3	AAA	201	CYC	NC-C4C-CHD-C1D
3	AAA	201	CYC	C3C-C4C-CHD-C1D
3	BBB	202	CYC	NA-C4A-CHB-C1B
3	BBB	202	CYC	C3A-C4A-CHB-C1B
3	CCC	201	CYC	NA-C4A-CHB-C1B
3	CCC	201	CYC	C3A-C4A-CHB-C1B
3	DDD	202	CYC	NA-C4A-CHB-C1B
3	DDD	202	CYC	C3A-C4A-CHB-C1B
3	DDD	203	CYC	NA-C4A-CHB-C1B
3	DDD	203	CYC	C3A-C4A-CHB-C1B
3	EEE	201	CYC	NA-C4A-CHB-C1B
3	EEE	201	CYC	C3A-C4A-CHB-C1B
3	FFF	503	CYC	NA-C4A-CHB-C1B
3	FFF	503	CYC	C3A-C4A-CHB-C1B
3	FFF	504	CYC	C3A-C4A-CHB-C1B
3	GGG	201	CYC	NA-C4A-CHB-C1B
3	GGG	201	CYC	C3A-C4A-CHB-C1B
3	GGG	201	CYC	NC-C4C-CHD-C1D
3	GGG	201	CYC	C3C-C4C-CHD-C1D
3	HHH	202	CYC	NA-C4A-CHB-C1B
3	HHH	202	CYC	C3A-C4A-CHB-C1B
3	HHH	202	CYC	C2B-C3B-CAB-CBB
3	HHH	202	CYC	C4B-C3B-CAB-CBB
3	HHH	203	CYC	C3A-C4A-CHB-C1B
3	HHH	203	CYC	C2B-C1B-CHB-C4A
3	III	201	CYC	NA-C4A-CHB-C1B
3	III	201	CYC	C2C-C3C-CAC-CBC
3	III	201	CYC	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
3	III	201	CYC	NC-C4C-CHD-C1D
3	JJJ	202	CYC	NA-C4A-CHB-C1B
3	JJJ	202	CYC	C3A-C4A-CHB-C1B
3	JJJ	202	CYC	C2B-C3B-CAB-CBB
3	JJJ	202	CYC	C4B-C3B-CAB-CBB
3	JJJ	203	CYC	C2B-C1B-CHB-C4A
3	JJJ	203	CYC	C2C-C3C-CAC-CBC
3	JJJ	203	CYC	C4C-C3C-CAC-CBC
3	KKK	201	CYC	NA-C4A-CHB-C1B
3	KKK	201	CYC	C3A-C4A-CHB-C1B
3	KKK	201	CYC	NC-C4C-CHD-C1D
3	LLL	202	CYC	NA-C4A-CHB-C1B
3	LLL	202	CYC	C3A-C4A-CHB-C1B
3	LLL	203	CYC	NA-C4A-CHB-C1B
3	LLL	203	CYC	C3A-C4A-CHB-C1B
3	LLL	203	CYC	C2C-C3C-CAC-CBC
3	LLL	203	CYC	C4C-C3C-CAC-CBC
3	BBB	202	CYC	C2B-C3B-CAB-CBB
3	DDD	202	CYC	C2B-C3B-CAB-CBB
3	FFF	503	CYC	C2B-C3B-CAB-CBB
3	FFF	504	CYC	C2B-C3B-CAB-CBB
3	EEE	201	CYC	C2B-C3B-CAB-CBB
3	JJJ	203	CYC	C2B-C3B-CAB-CBB
3	GGG	201	CYC	ND-C1D-CHD-C4C
3	III	201	CYC	ND-C1D-CHD-C4C
3	BBB	202	CYC	C2D-C1D-CHD-C4C
3	CCC	201	CYC	C2D-C1D-CHD-C4C
3	DDD	203	CYC	C2D-C1D-CHD-C4C
3	GGG	201	CYC	C2D-C1D-CHD-C4C
3	HHH	203	CYC	C2D-C1D-CHD-C4C
3	III	201	CYC	C2D-C1D-CHD-C4C
3	JJJ	203	CYC	C2D-C1D-CHD-C4C
3	HHH	203	CYC	NB-C1B-CHB-C4A
3	JJJ	203	CYC	NB-C1B-CHB-C4A
3	III	201	CYC	C3A-C4A-CHB-C1B
3	AAA	201	CYC	ND-C1D-CHD-C4C
3	BBB	202	CYC	ND-C1D-CHD-C4C
3	BBB	203	CYC	ND-C1D-CHD-C4C
3	CCC	201	CYC	ND-C1D-CHD-C4C
3	DDD	202	CYC	ND-C1D-CHD-C4C
3	DDD	203	CYC	ND-C1D-CHD-C4C
3	EEE	201	CYC	ND-C1D-CHD-C4C

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Mol	Chain	Res	Type	Atoms
3	FFF	503	CYC	ND-C1D-CHD-C4C
3	FFF	504	CYC	ND-C1D-CHD-C4C
3	HHH	202	CYC	ND-C1D-CHD-C4C
3	HHH	203	CYC	ND-C1D-CHD-C4C
3	JJJ	203	CYC	ND-C1D-CHD-C4C
3	KKK	201	CYC	ND-C1D-CHD-C4C
3	LLL	202	CYC	ND-C1D-CHD-C4C
3	LLL	203	CYC	ND-C1D-CHD-C4C
3	AAA	201	CYC	C2D-C1D-CHD-C4C
3	BBB	203	CYC	C2D-C1D-CHD-C4C
3	DDD	202	CYC	C2D-C1D-CHD-C4C
3	EEE	201	CYC	C2D-C1D-CHD-C4C
3	FFF	503	CYC	C2D-C1D-CHD-C4C
3	FFF	504	CYC	C2D-C1D-CHD-C4C
3	HHH	202	CYC	C2D-C1D-CHD-C4C
3	KKK	201	CYC	C2D-C1D-CHD-C4C
3	LLL	202	CYC	C2D-C1D-CHD-C4C
3	LLL	203	CYC	C2D-C1D-CHD-C4C
3	FFF	504	CYC	NB-C1B-CHB-C4A
3	JJJ	202	CYC	ND-C1D-CHD-C4C
3	JJJ	202	CYC	C2D-C1D-CHD-C4C
3	BBB	202	CYC	C4B-C3B-CAB-CBB
3	DDD	202	CYC	C4B-C3B-CAB-CBB
3	FFF	503	CYC	C4B-C3B-CAB-CBB
3	FFF	504	CYC	C4B-C3B-CAB-CBB
3	FFF	504	CYC	C2B-C1B-CHB-C4A
3	BBB	203	CYC	NA-C4A-CHB-C1B
3	FFF	504	CYC	NA-C4A-CHB-C1B
3	HHH	203	CYC	NA-C4A-CHB-C1B
3	JJJ	203	CYC	NA-C4A-CHB-C1B
3	LLL	203	CYC	NB-C1B-CHB-C4A
3	BBB	203	CYC	C3A-C4A-CHB-C1B
3	JJJ	203	CYC	C3A-C4A-CHB-C1B
3	EEE	201	CYC	C4B-C3B-CAB-CBB
3	JJJ	203	CYC	C4B-C3B-CAB-CBB
3	BBB	203	CYC	C2A-CAA-CBA-CGA
3	BBB	202	CYC	C2C-C3C-CAC-CBC
3	BBB	202	CYC	C2A-CAA-CBA-CGA
3	LLL	203	CYC	C2A-CAA-CBA-CGA
3	DDD	203	CYC	C4C-C3C-CAC-CBC
3	FFF	504	CYC	C4C-C3C-CAC-CBC
3	KKK	201	CYC	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
3	AAA	201	CYC	C2B-C3B-CAB-CBB
3	DDD	203	CYC	C2C-C3C-CAC-CBC
3	FFF	504	CYC	C2C-C3C-CAC-CBC
3	HHH	202	CYC	C2C-C3C-CAC-CBC
3	GGG	201	CYC	C2B-C3B-CAB-CBB
3	GGG	201	CYC	CAA-CBA-CGA-O2A
3	DDD	202	CYC	CAA-CBA-CGA-O2A
3	BBB	203	CYC	CAA-CBA-CGA-O2A
3	JJJ	203	CYC	CAA-CBA-CGA-O2A
3	KKK	201	CYC	CAA-CBA-CGA-O1A
3	AAA	201	CYC	CAA-CBA-CGA-O2A
3	DDD	203	CYC	CAA-CBA-CGA-O1A
3	LLL	203	CYC	C2B-C1B-CHB-C4A
3	GGG	201	CYC	CAA-CBA-CGA-O1A
3	LLL	202	CYC	CAA-CBA-CGA-O2A
3	FFF	503	CYC	CAA-CBA-CGA-O1A
3	HHH	202	CYC	CAA-CBA-CGA-O1A
3	III	201	CYC	CAA-CBA-CGA-O1A
3	HHH	202	CYC	CAA-CBA-CGA-O2A
3	EEE	201	CYC	CAA-CBA-CGA-O2A
3	HHH	203	CYC	CAD-CBD-CGD-O1D
3	JJJ	203	CYC	CAA-CBA-CGA-O1A
3	KKK	201	CYC	CAA-CBA-CGA-O2A
3	AAA	201	CYC	CAA-CBA-CGA-O1A
3	FFF	503	CYC	CAD-CBD-CGD-O1D
3	DDD	202	CYC	CAA-CBA-CGA-O1A
3	FFF	503	CYC	CAA-CBA-CGA-O2A
3	LLL	203	CYC	CAD-CBD-CGD-O1D
3	BBB	203	CYC	CAA-CBA-CGA-O1A
3	DDD	203	CYC	CAA-CBA-CGA-O2A
3	III	201	CYC	CAA-CBA-CGA-O2A
3	LLL	202	CYC	CAA-CBA-CGA-O1A
3	EEE	201	CYC	CAA-CBA-CGA-O1A
3	HHH	203	CYC	CAD-CBD-CGD-O2D
3	LLL	203	CYC	CAD-CBD-CGD-O2D
3	LLL	203	CYC	CAA-CBA-CGA-O2A
3	LLL	203	CYC	CAA-CBA-CGA-O1A
3	FFF	504	CYC	CAA-CBA-CGA-O2A
3	JJJ	202	CYC	CAA-CBA-CGA-O1A
3	CCC	201	CYC	CAA-CBA-CGA-O2A
3	EEE	201	CYC	NA-C1A-CHA-C4D
3	DDD	203	CYC	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
3	FFF	504	CYC	CAD-CBD-CGD-O1D
3	CCC	201	CYC	CAA-CBA-CGA-O1A
3	FFF	504	CYC	C2D-C3D-CAD-CBD
3	FFF	504	CYC	CAA-CBA-CGA-O1A
3	LLL	202	CYC	C2B-C3B-CAB-CBB
3	GGG	201	CYC	CAD-CBD-CGD-O1D
3	JJJ	202	CYC	CAA-CBA-CGA-O2A
3	BBB	202	CYC	CAD-CBD-CGD-O1D
3	BBB	203	CYC	CAD-CBD-CGD-O1D
3	FFF	503	CYC	CAD-CBD-CGD-O2D
3	BBB	202	CYC	CAD-CBD-CGD-O2D
3	GGG	201	CYC	CAD-CBD-CGD-O2D
3	BBB	202	CYC	CAA-CBA-CGA-O1A
3	FFF	504	CYC	CAD-CBD-CGD-O2D
3	CCC	201	CYC	C2B-C3B-CAB-CBB
3	HHH	203	CYC	CAA-CBA-CGA-O2A
3	HHH	203	CYC	CAA-CBA-CGA-O1A
3	FFF	504	CYC	C4D-C3D-CAD-CBD
3	KKK	201	CYC	CAD-CBD-CGD-O2D
3	EEE	201	CYC	C3C-C4C-CHD-C1D
3	KKK	201	CYC	C3C-C4C-CHD-C1D
3	BBB	202	CYC	CAA-CBA-CGA-O2A
3	BBB	203	CYC	CAD-CBD-CGD-O2D
3	HHH	202	CYC	CAD-CBD-CGD-O2D

There are no ring outliers.

20 monomers are involved in 140 short contacts:

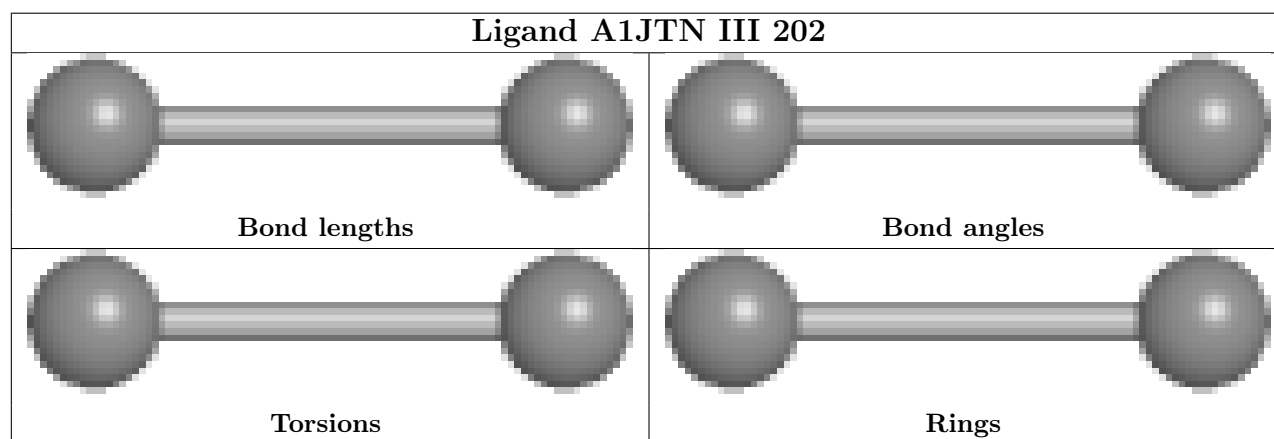
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	KKK	201	CYC	6	0
3	JJJ	202	CYC	9	0
3	BBB	202	CYC	7	0
3	CCC	201	CYC	6	0
3	GGG	201	CYC	8	0
3	BBB	203	CYC	7	0
3	LLL	202	CYC	7	0
4	LLL	201	A1JTN	1	0
3	HHH	202	CYC	12	0
3	HHH	203	CYC	7	0
3	DDD	202	CYC	10	0
3	JJJ	203	CYC	5	0
3	EEE	201	CYC	10	0

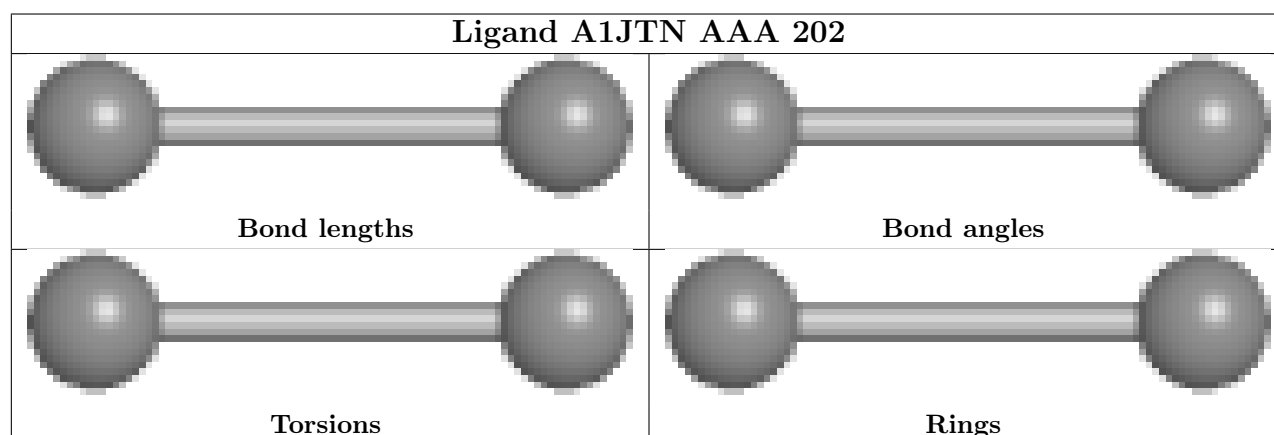
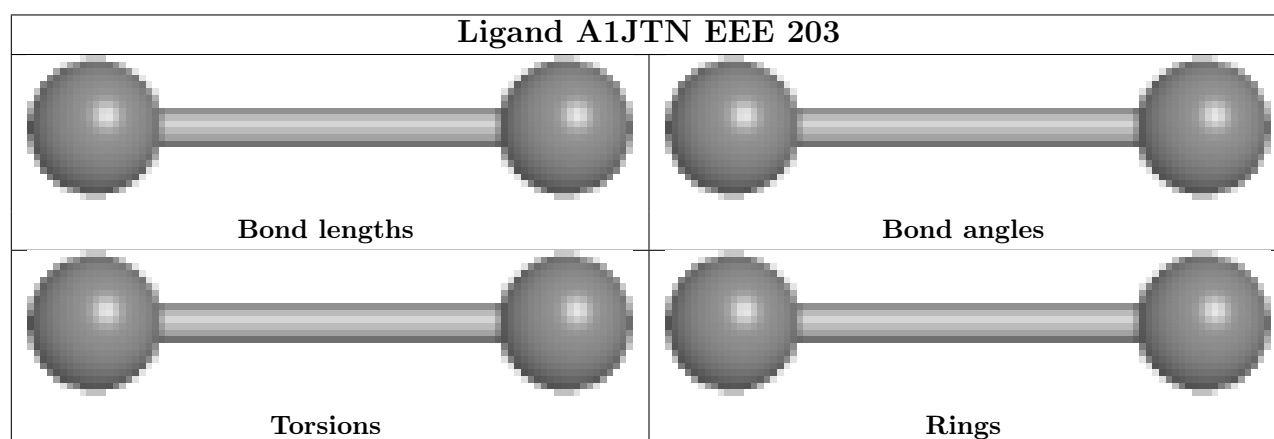
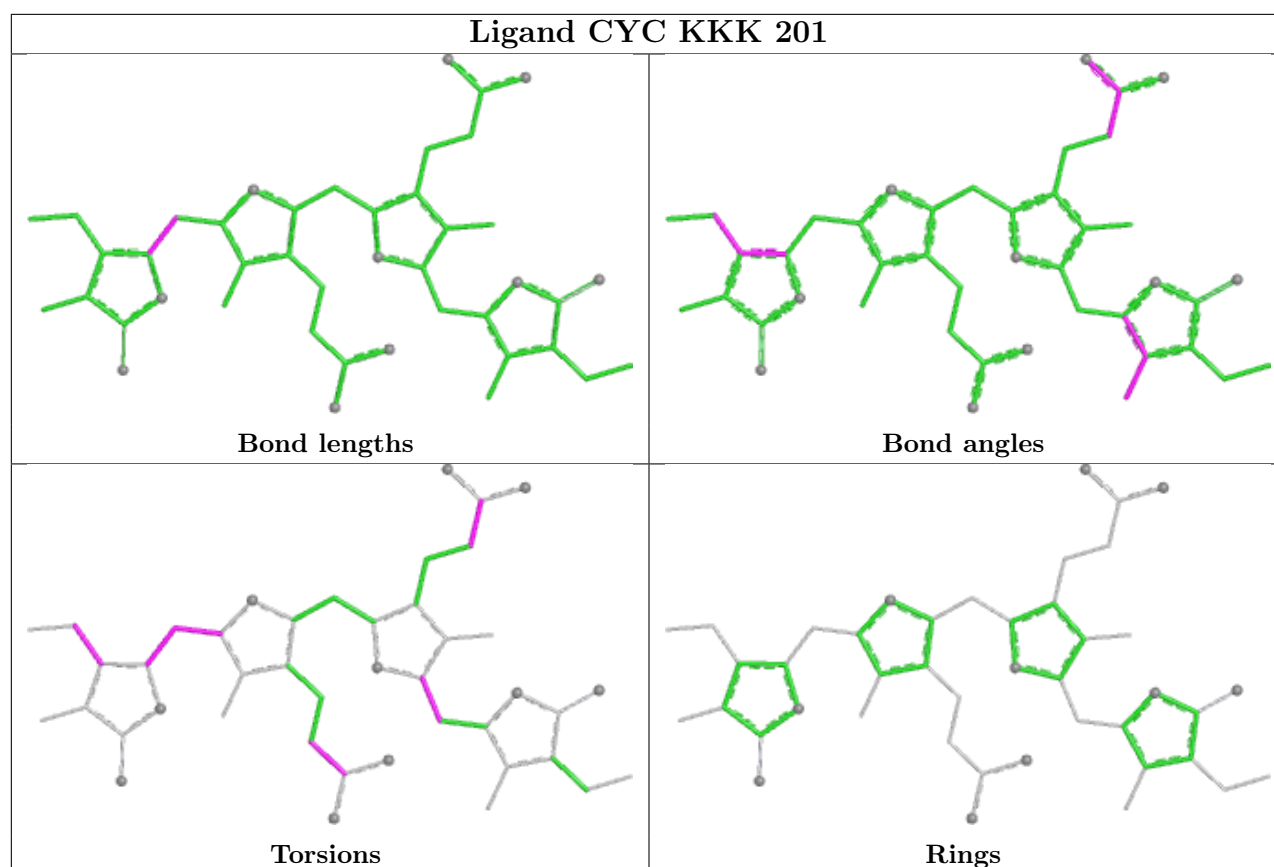
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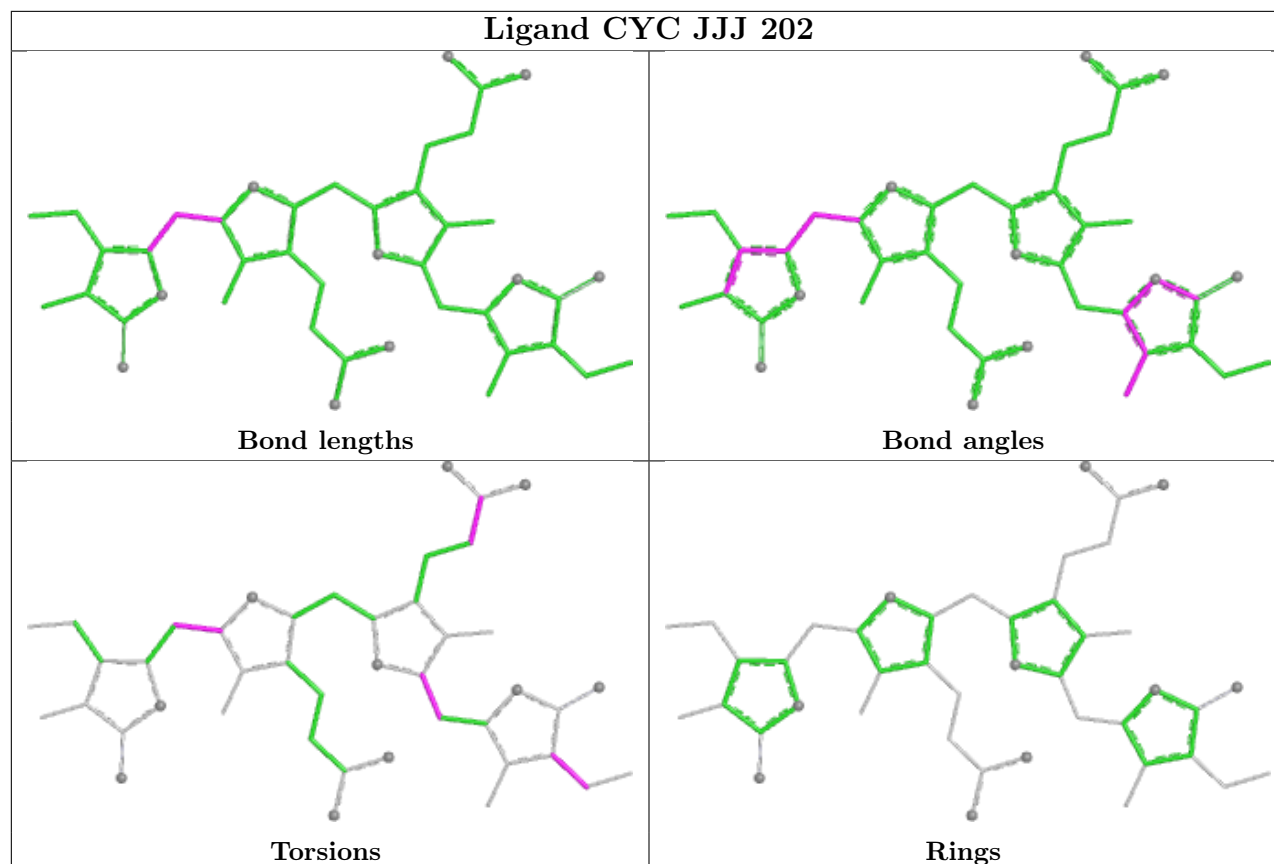
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	AAA	201	CYC	8	0
3	FFF	504	CYC	9	0
3	DDD	203	CYC	7	0
3	III	201	CYC	3	0
4	DDD	201	A1JTN	1	0
3	FFF	503	CYC	9	0
3	LLL	203	CYC	8	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

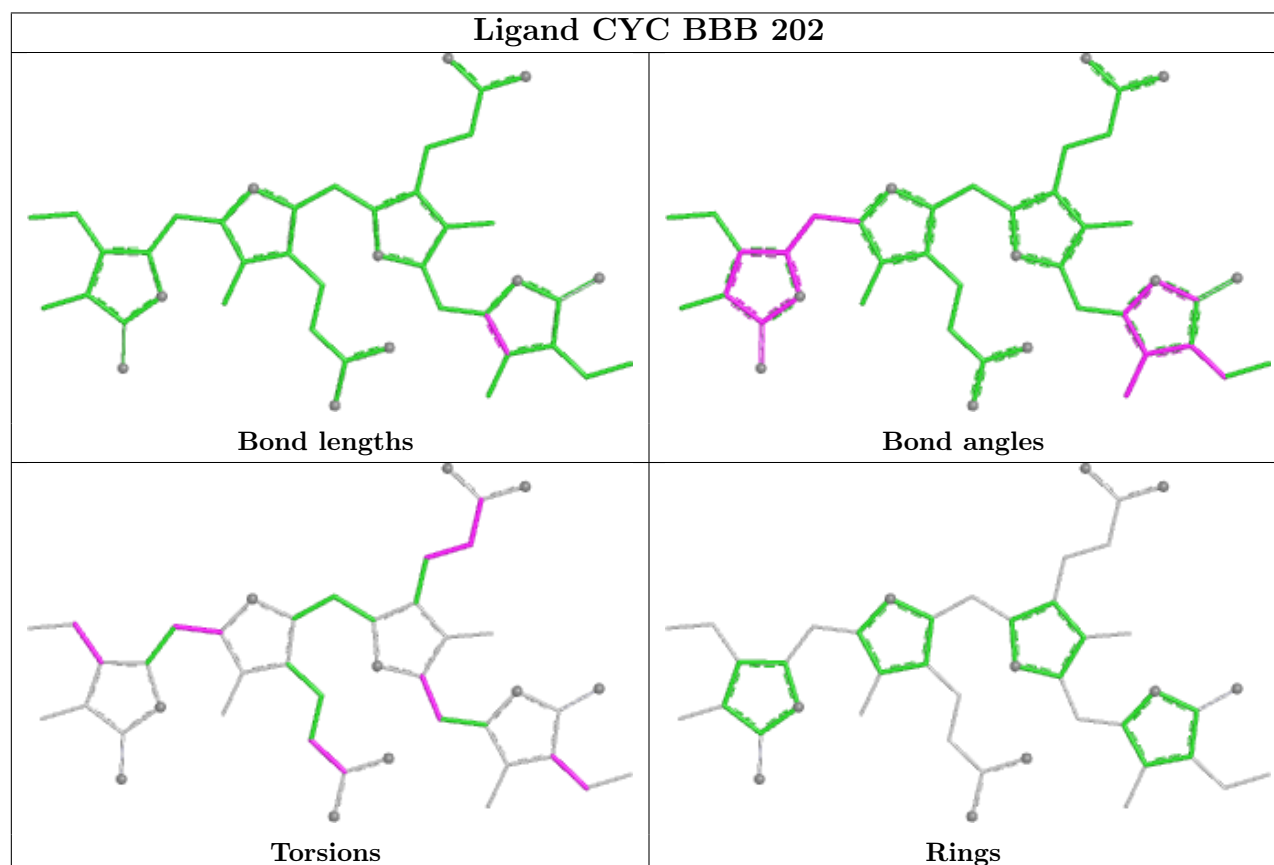




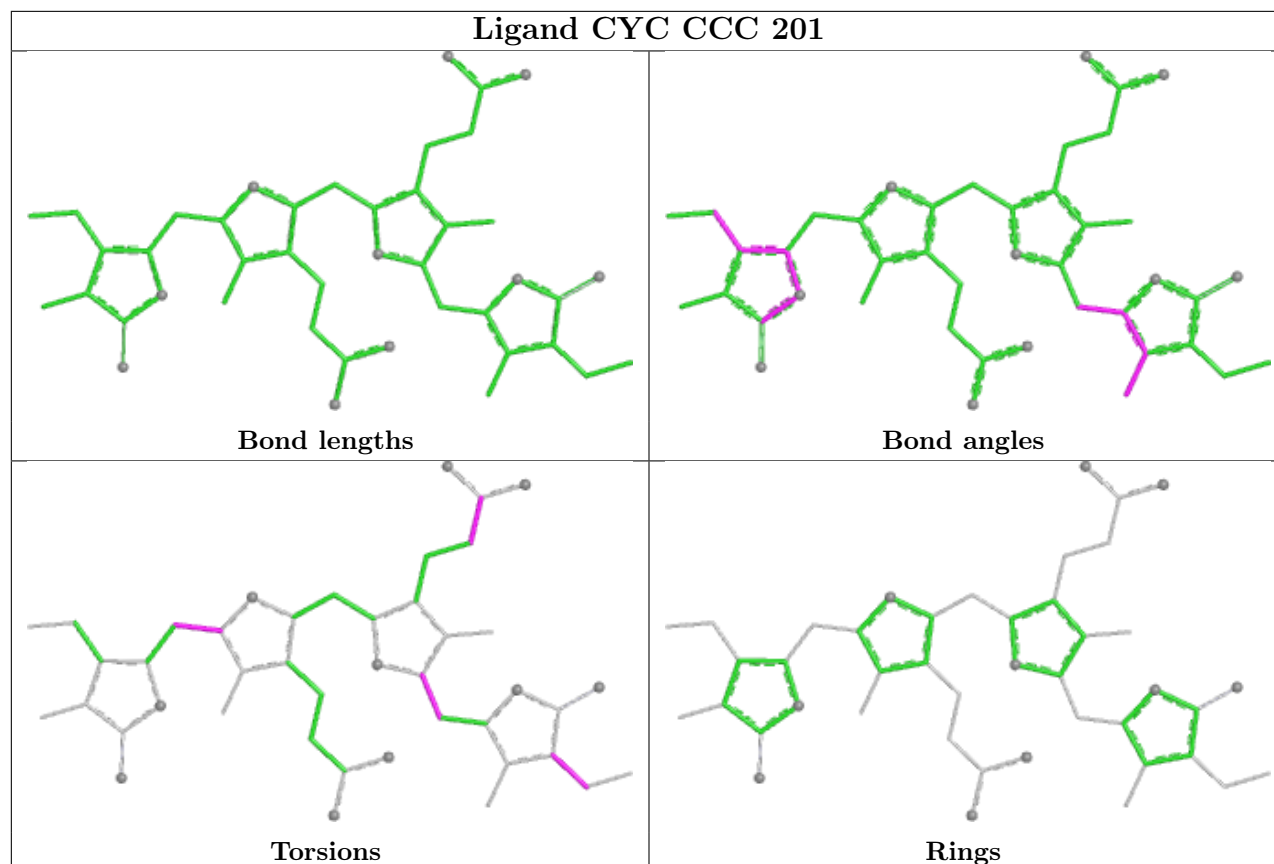
Ligand CYC JJJ 202



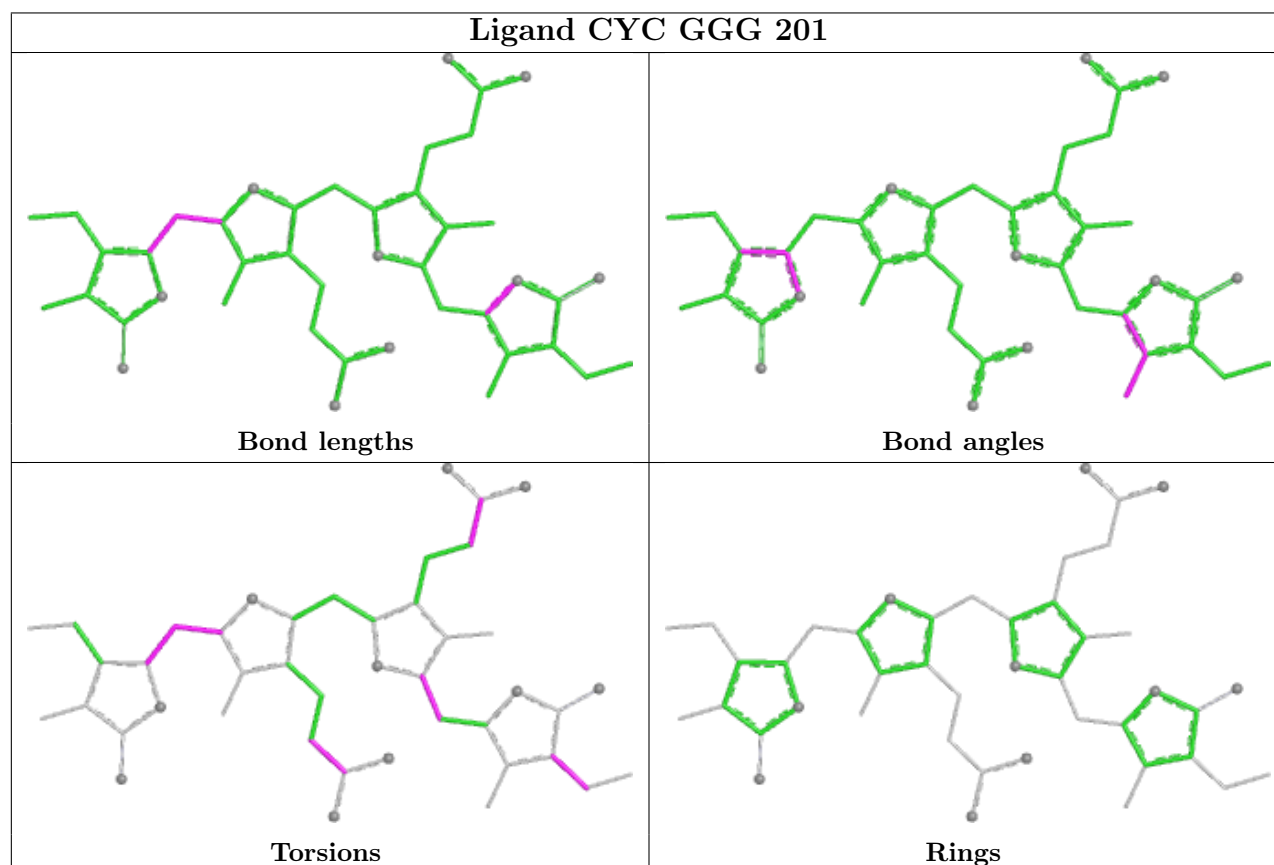
Ligand CYC BBB 202



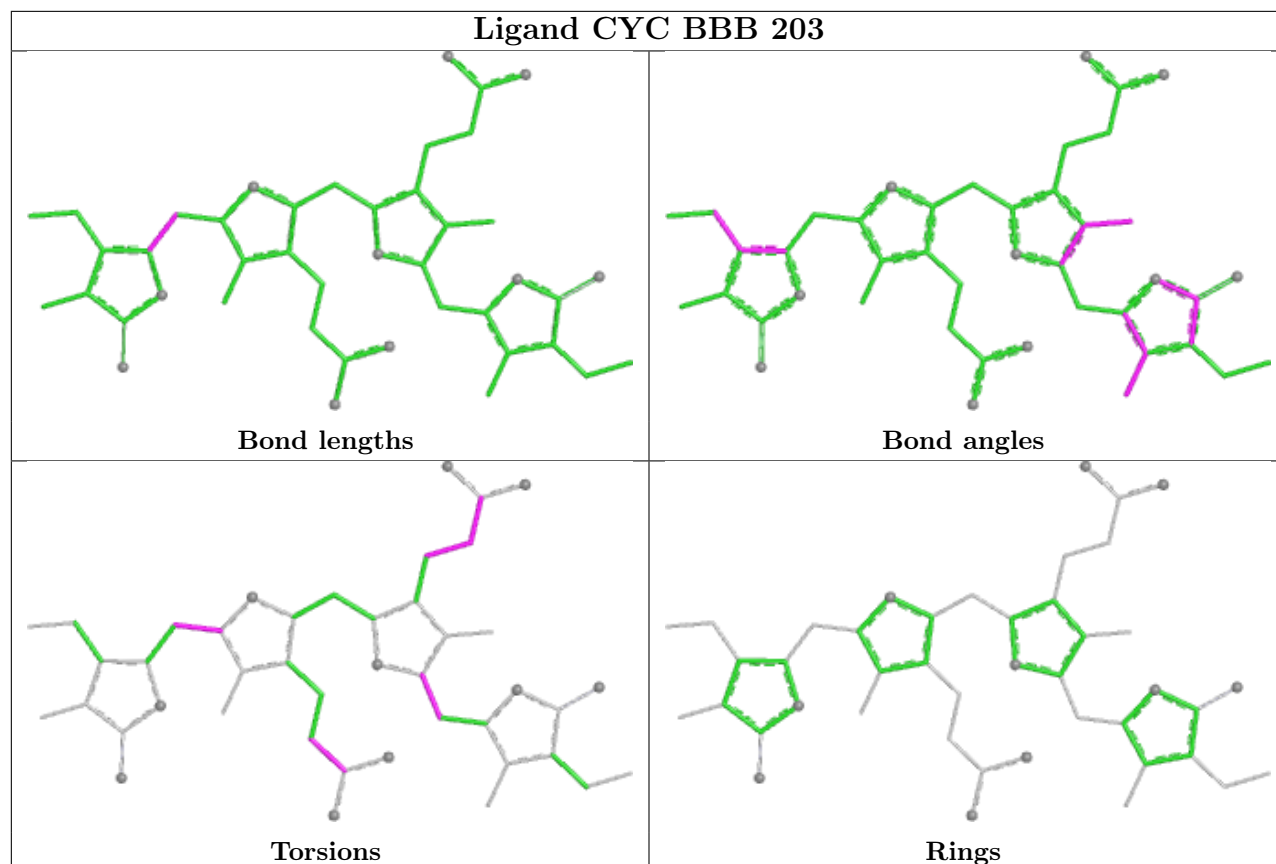
Ligand CYC CCC 201



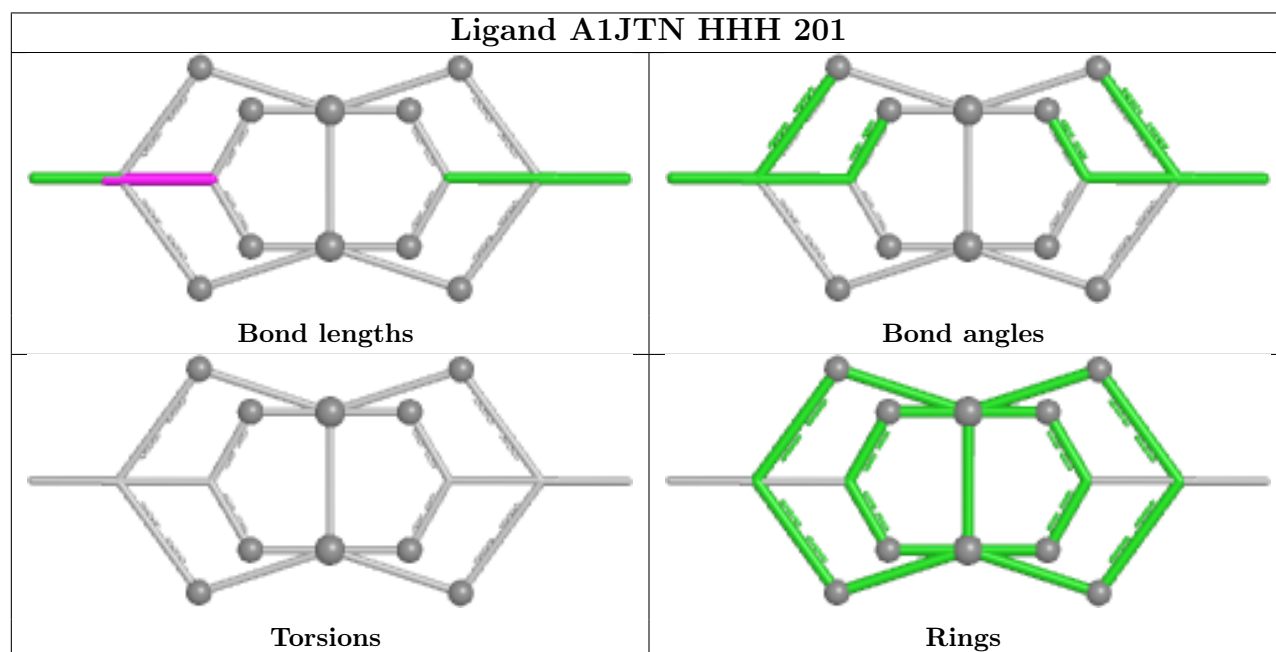
Ligand CYC GGG 201

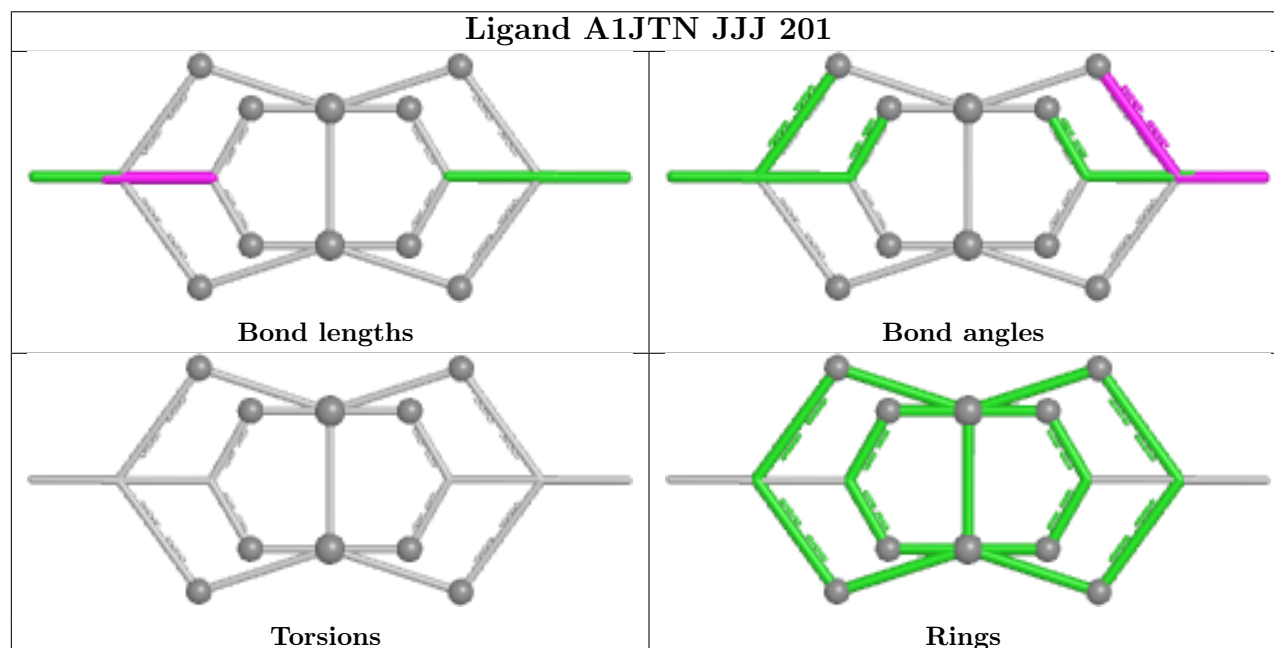
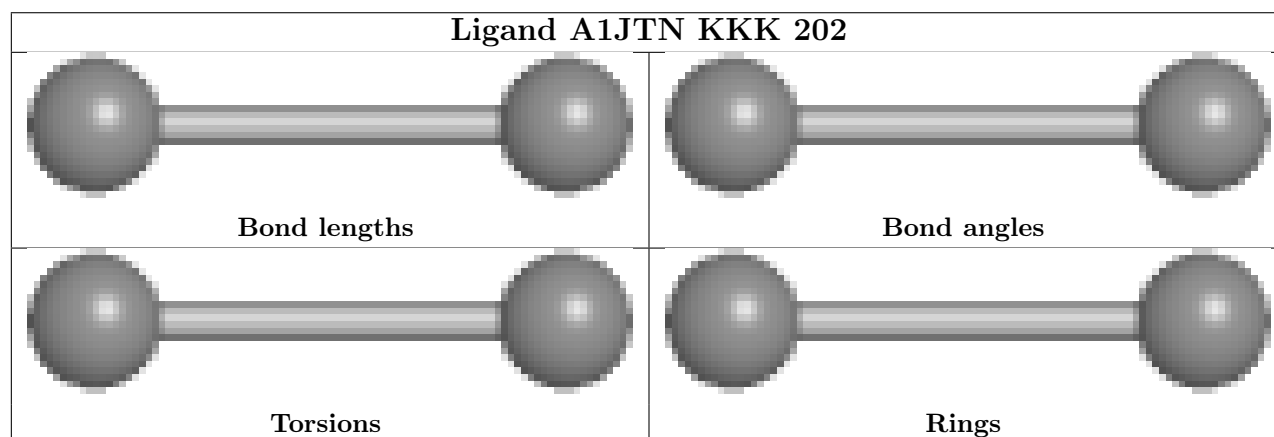
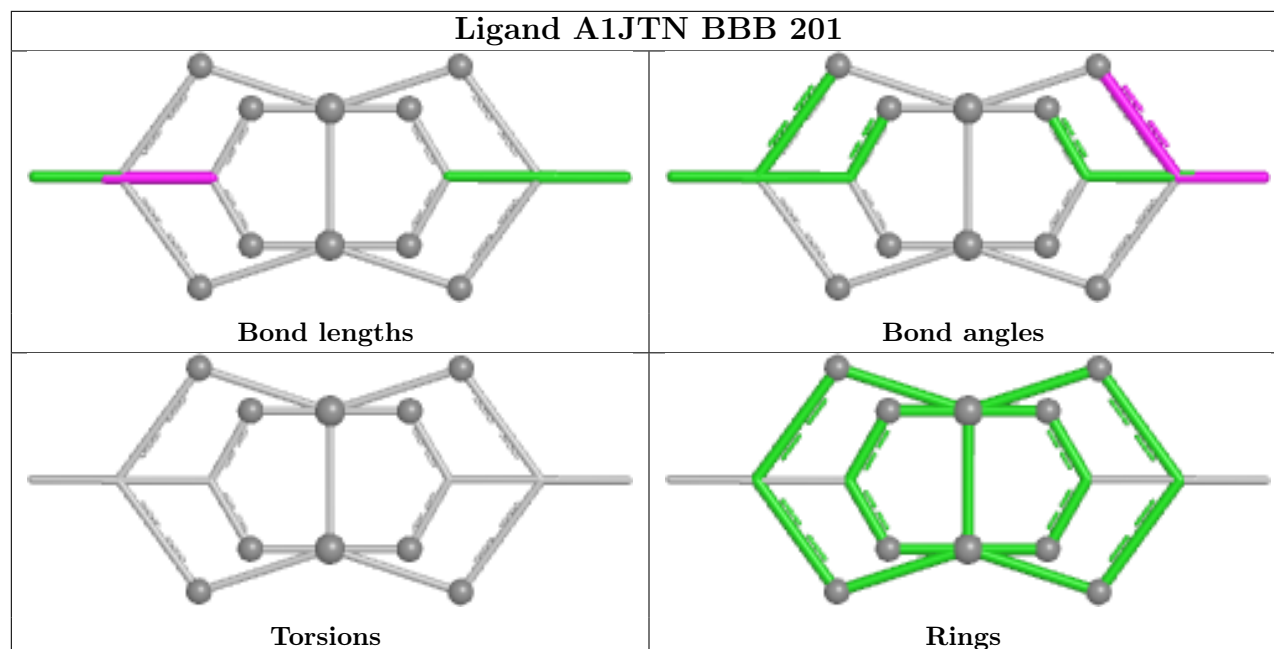


Ligand CYC BBB 203

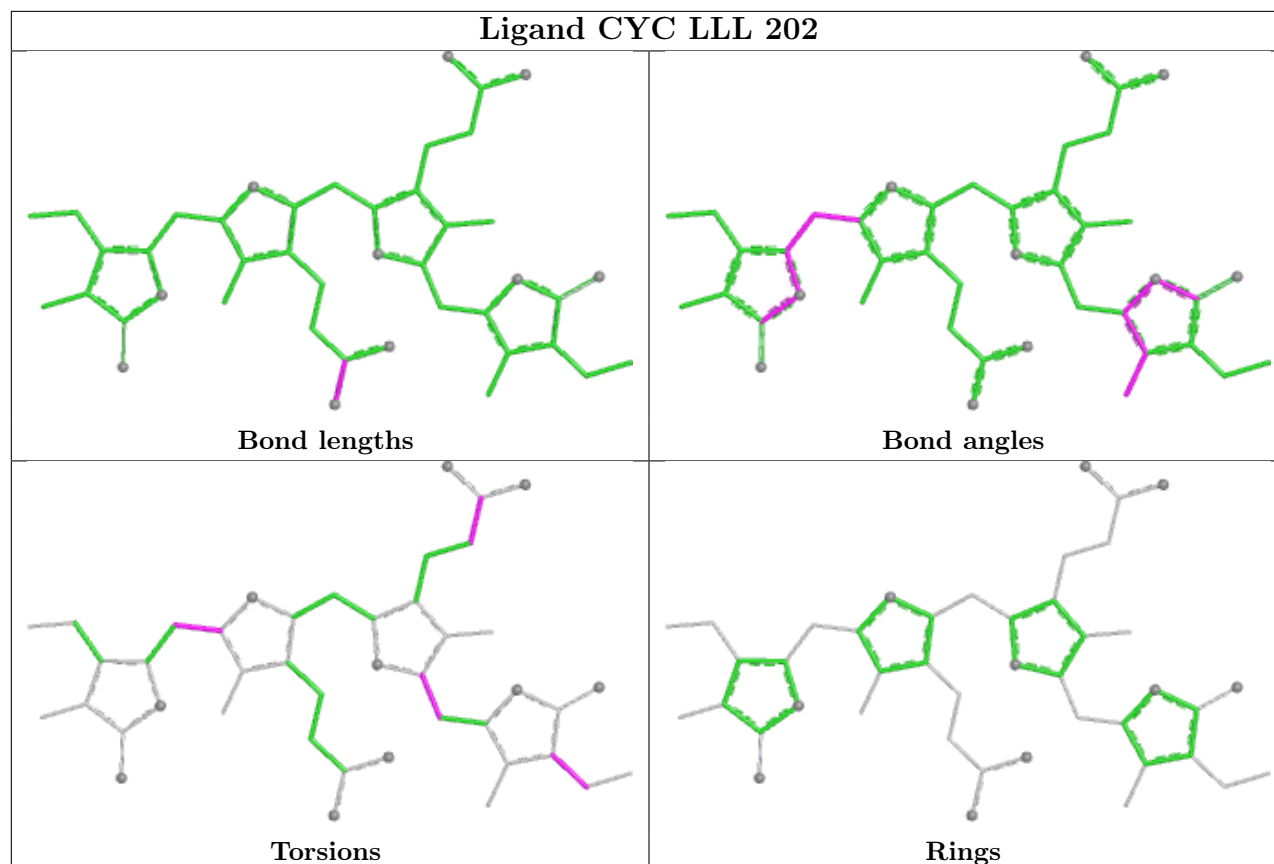


Ligand A1JTN HHH 201

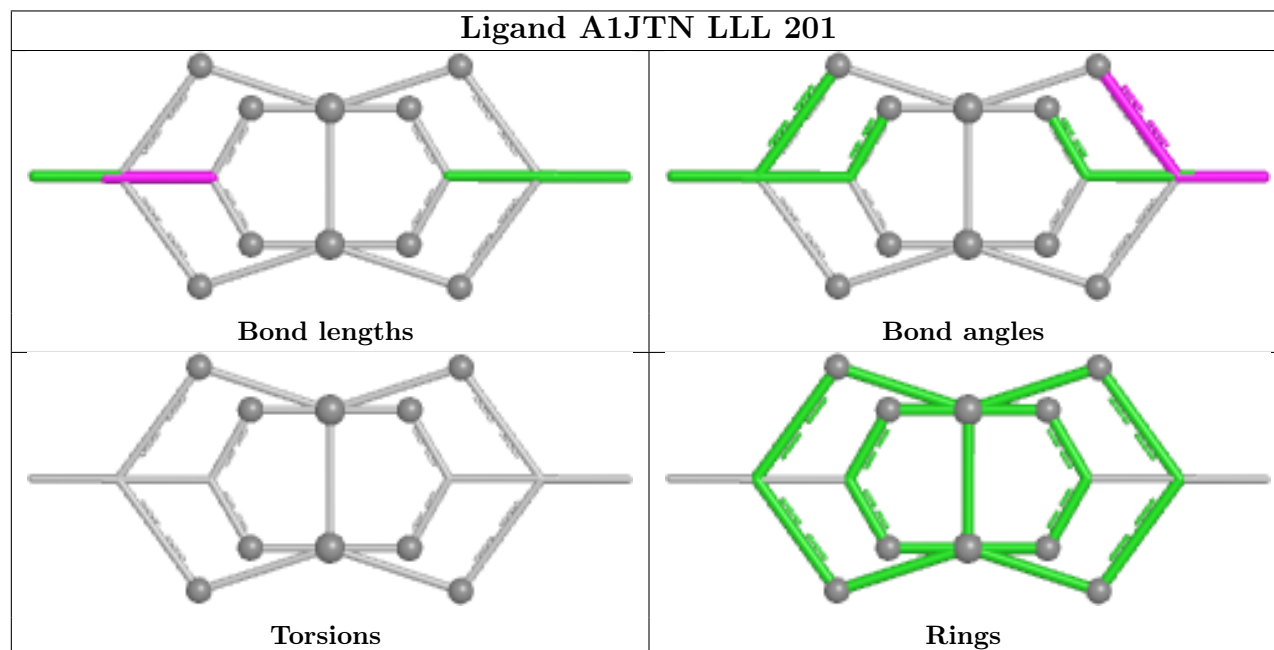




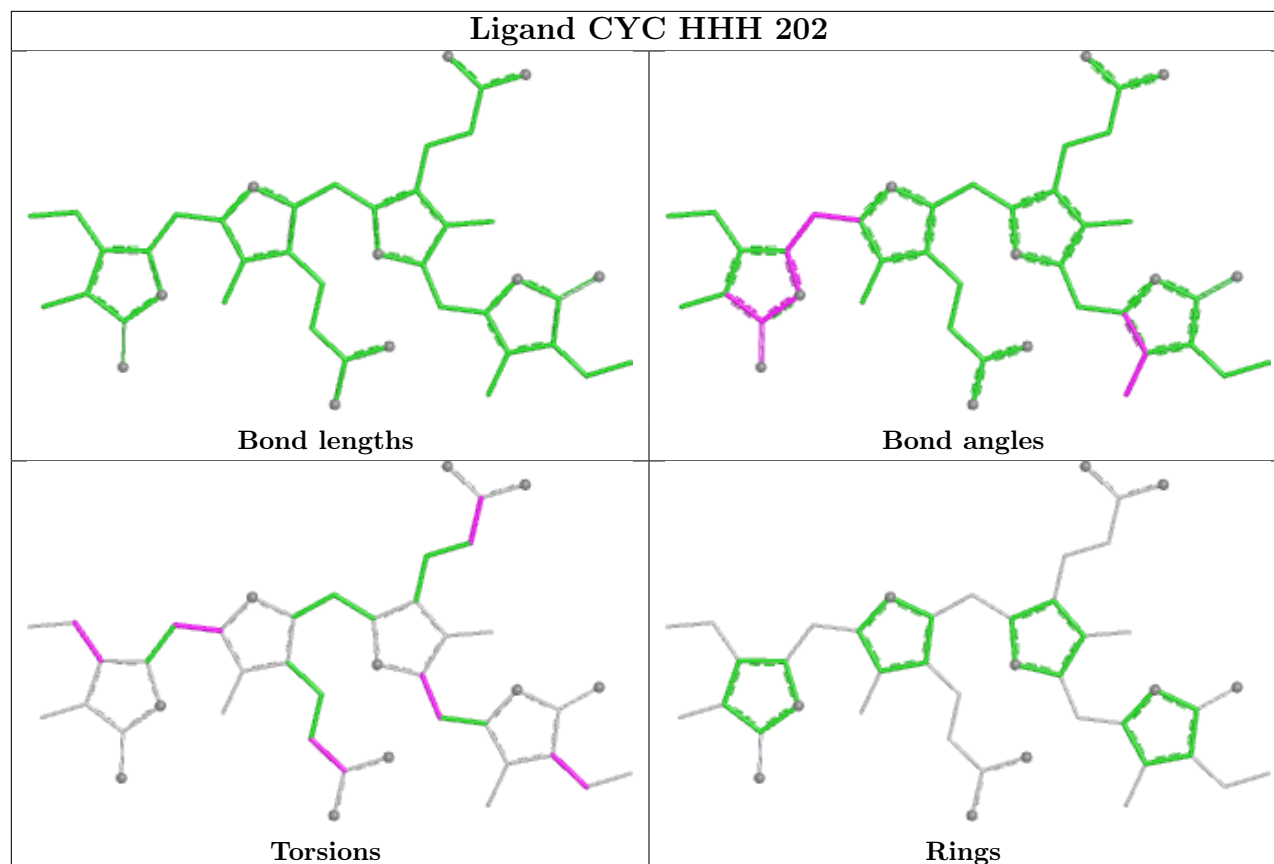
Ligand CYC LLL 202



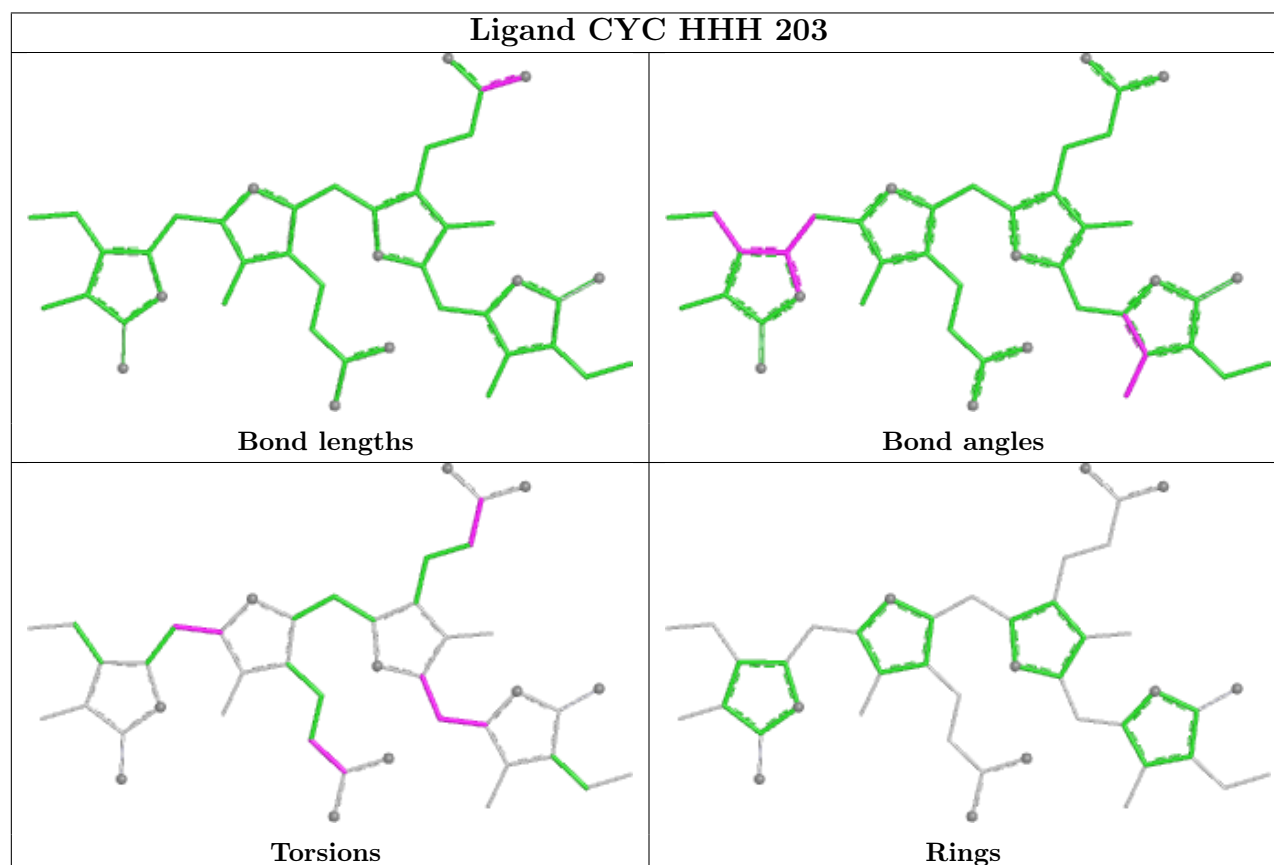
Ligand A1JTN LLL 201

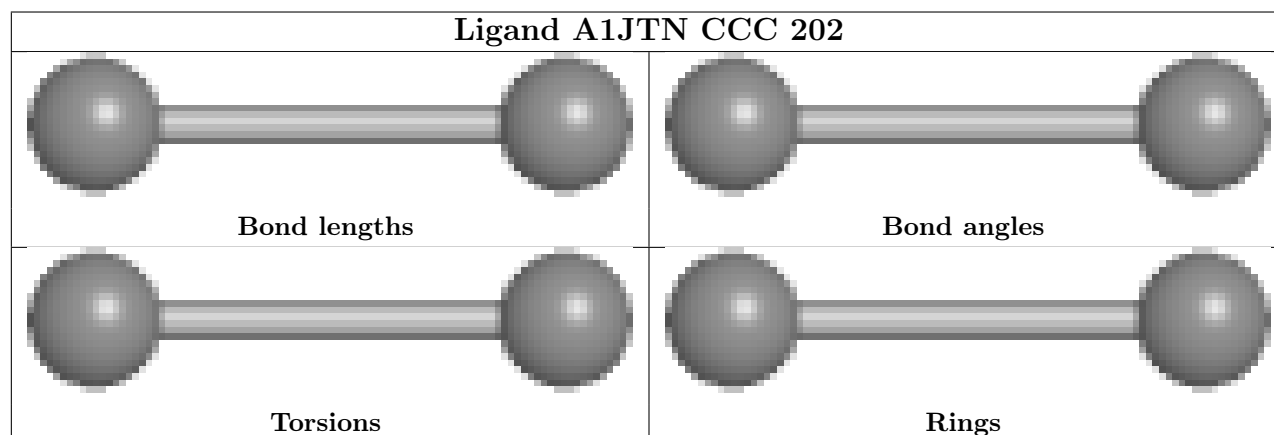
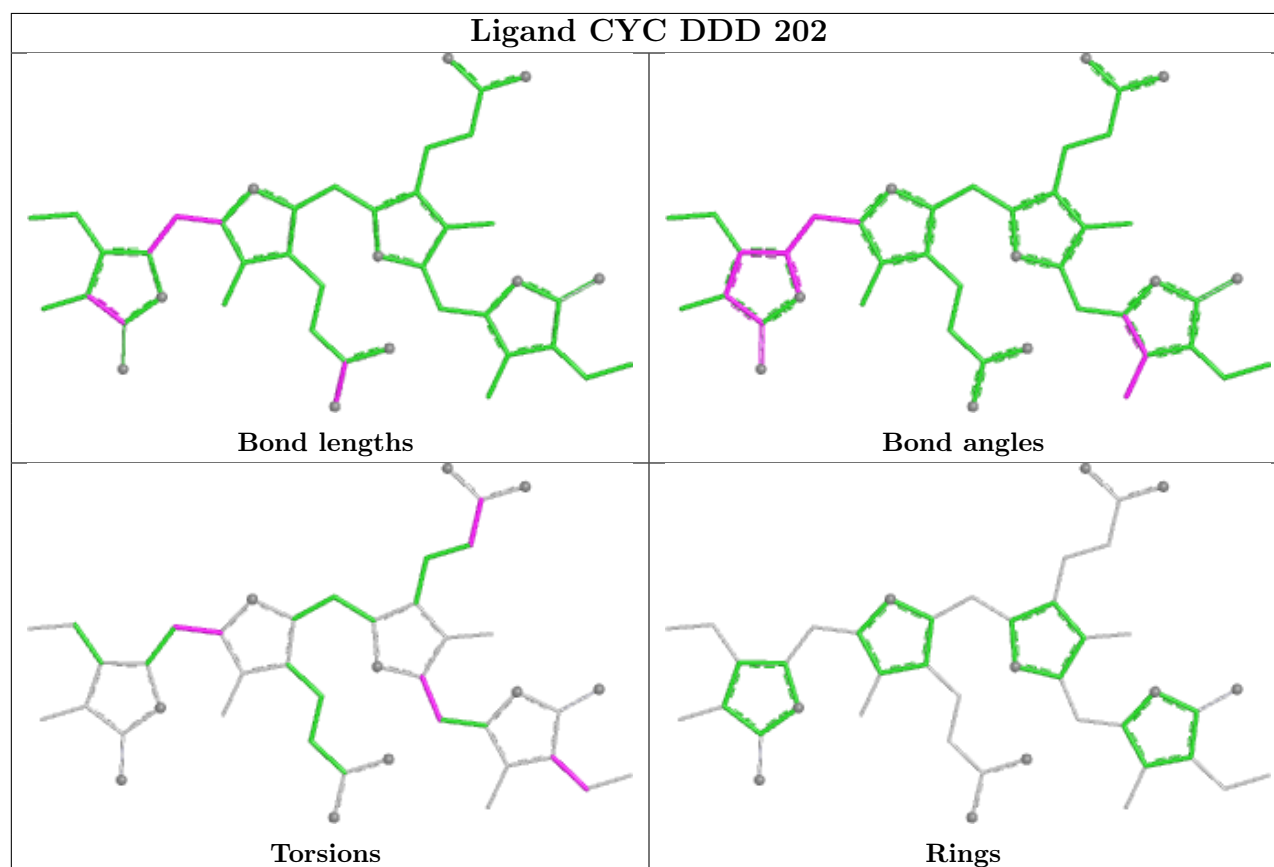
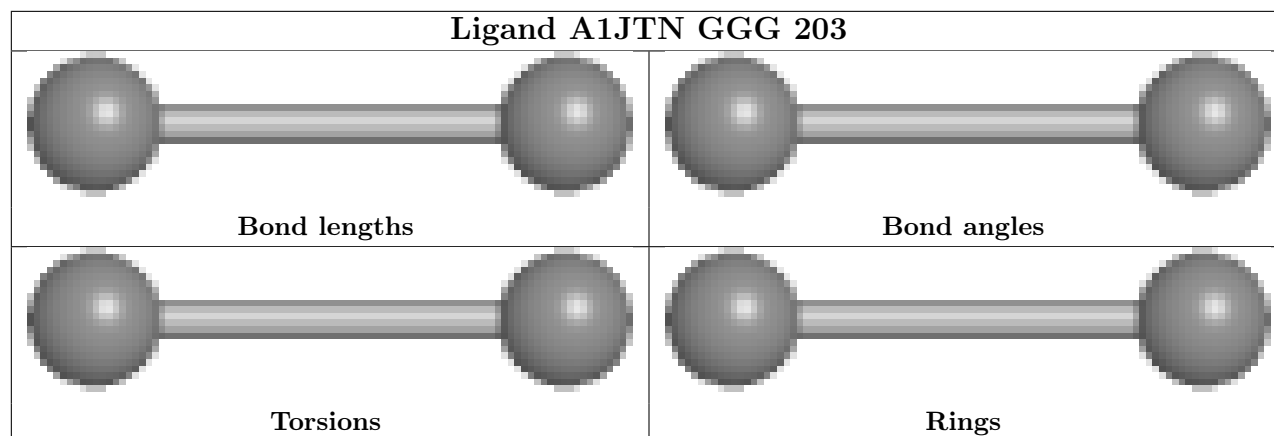


Ligand CYC HHH 202

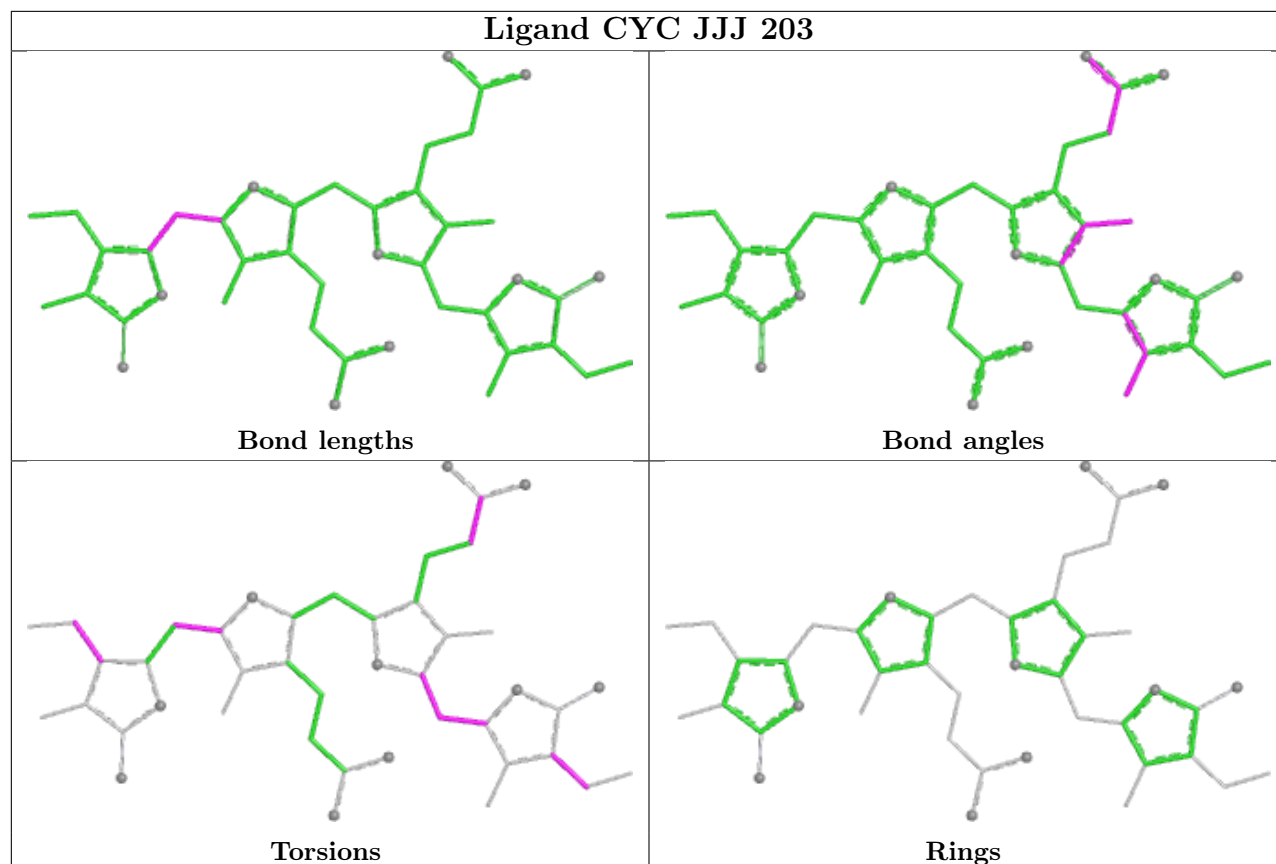


Ligand CYC HHH 203

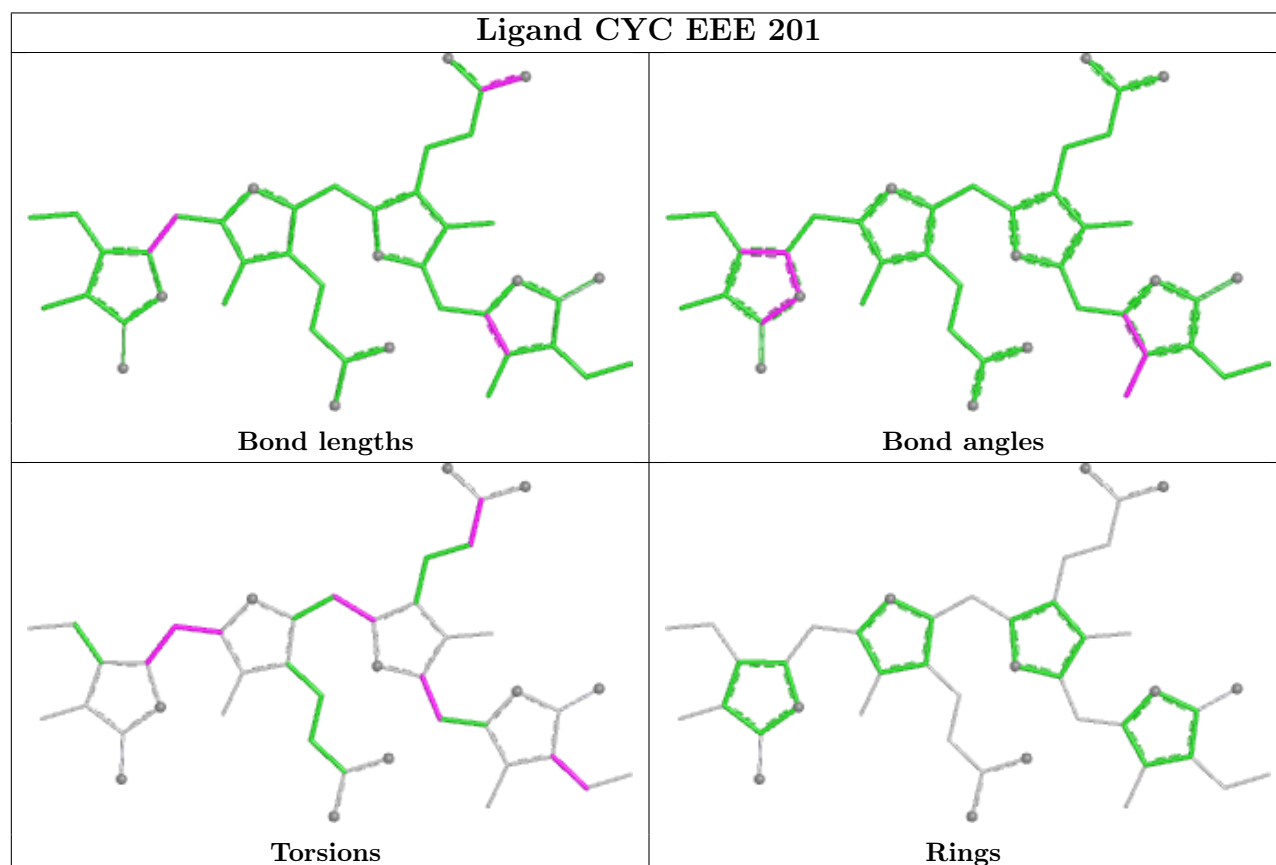


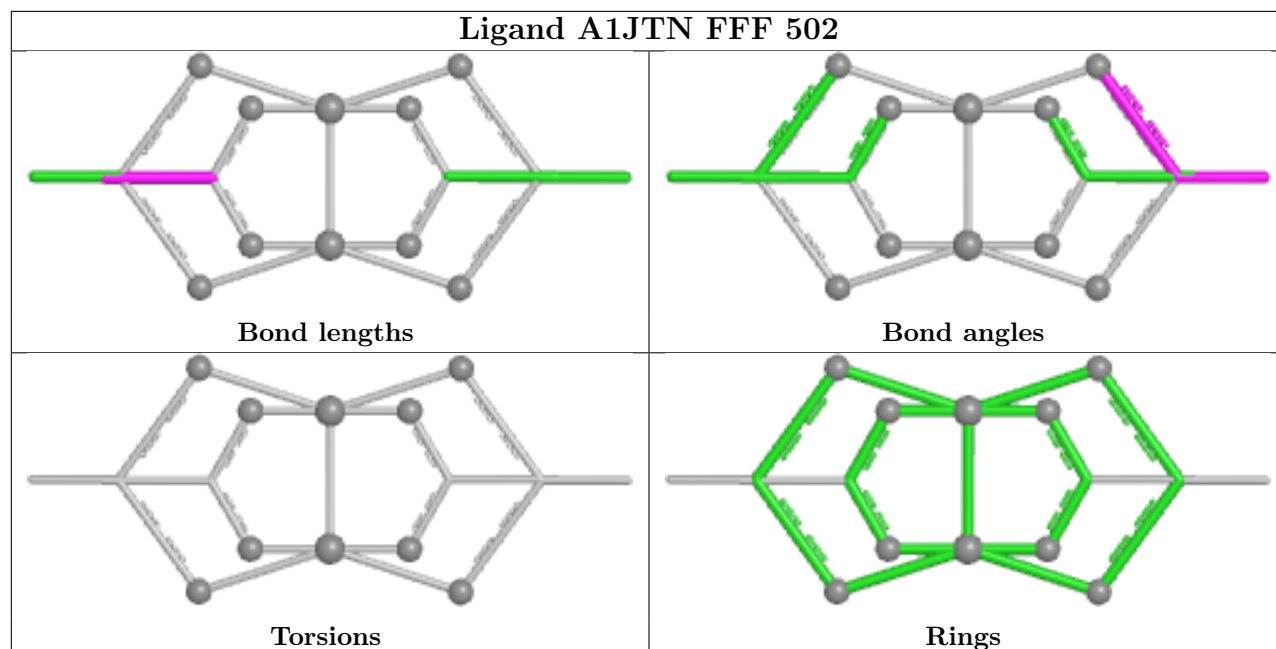
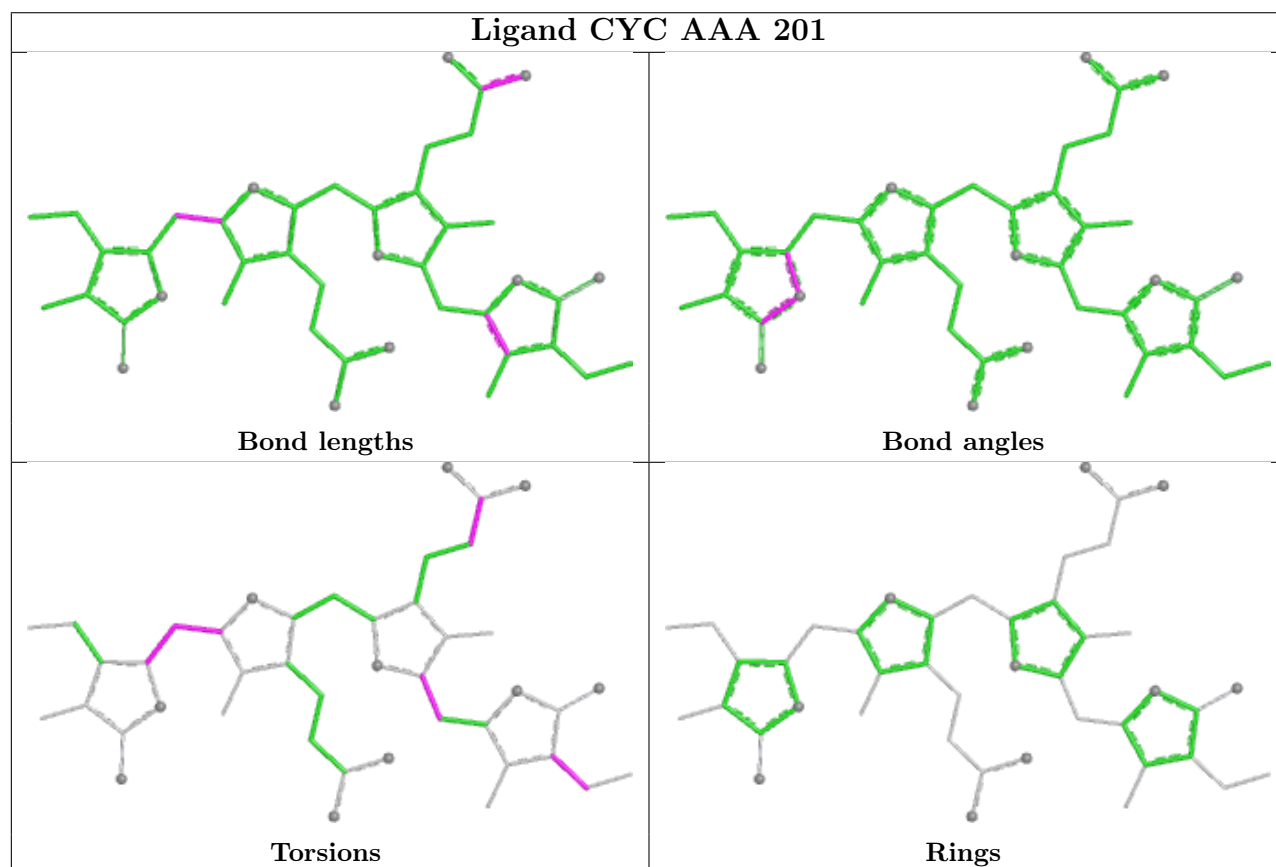


Ligand CYC JJJ 203

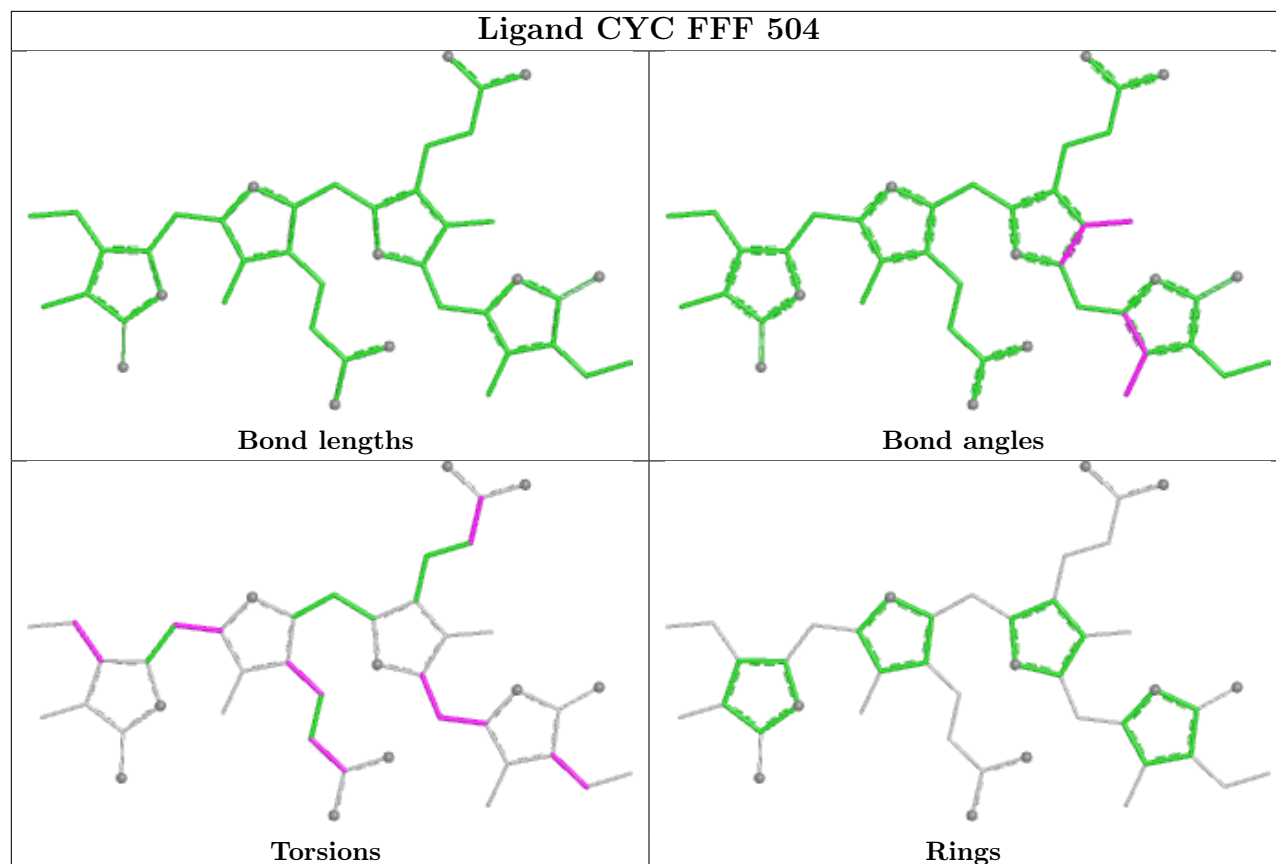


Ligand CYC EEE 201

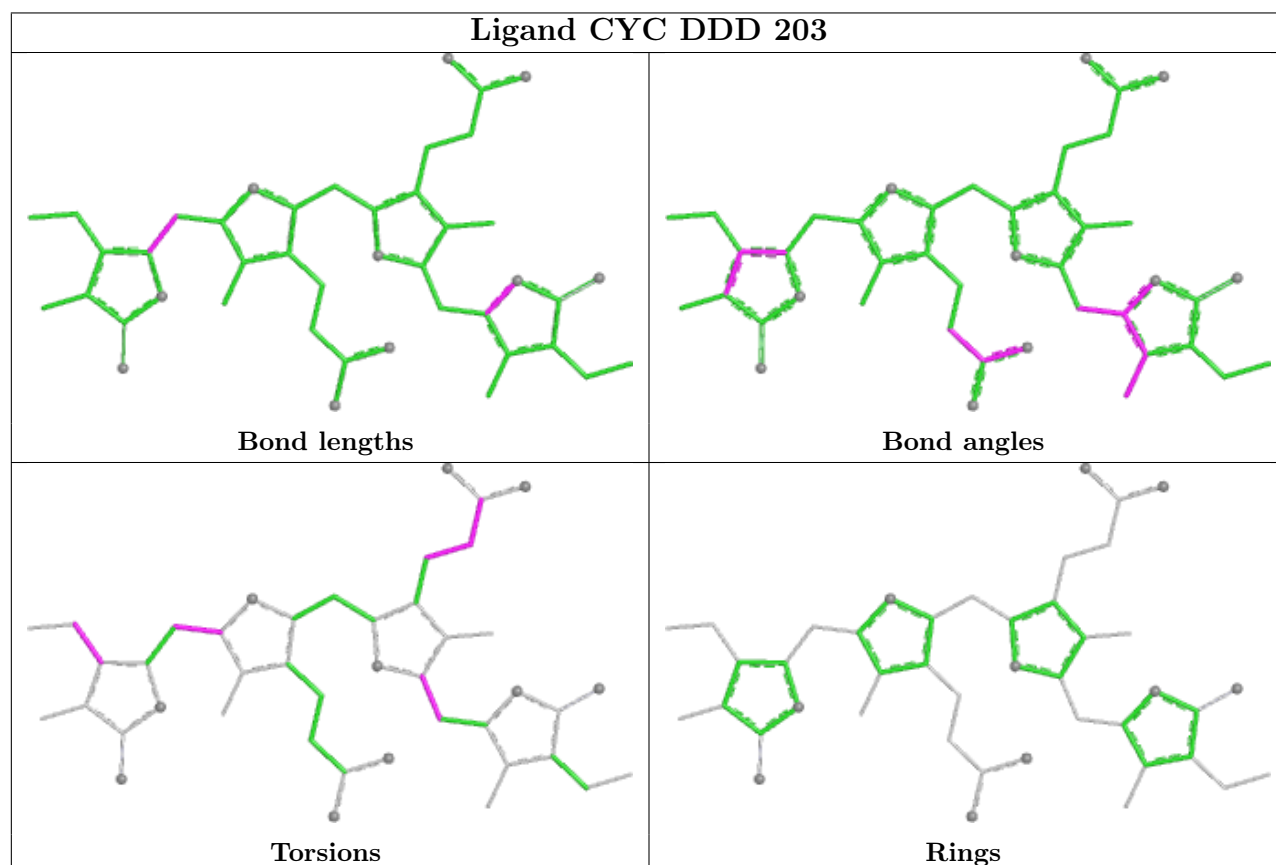


Ligand A1JTN FFF 502**Ligand CYC AAA 201**

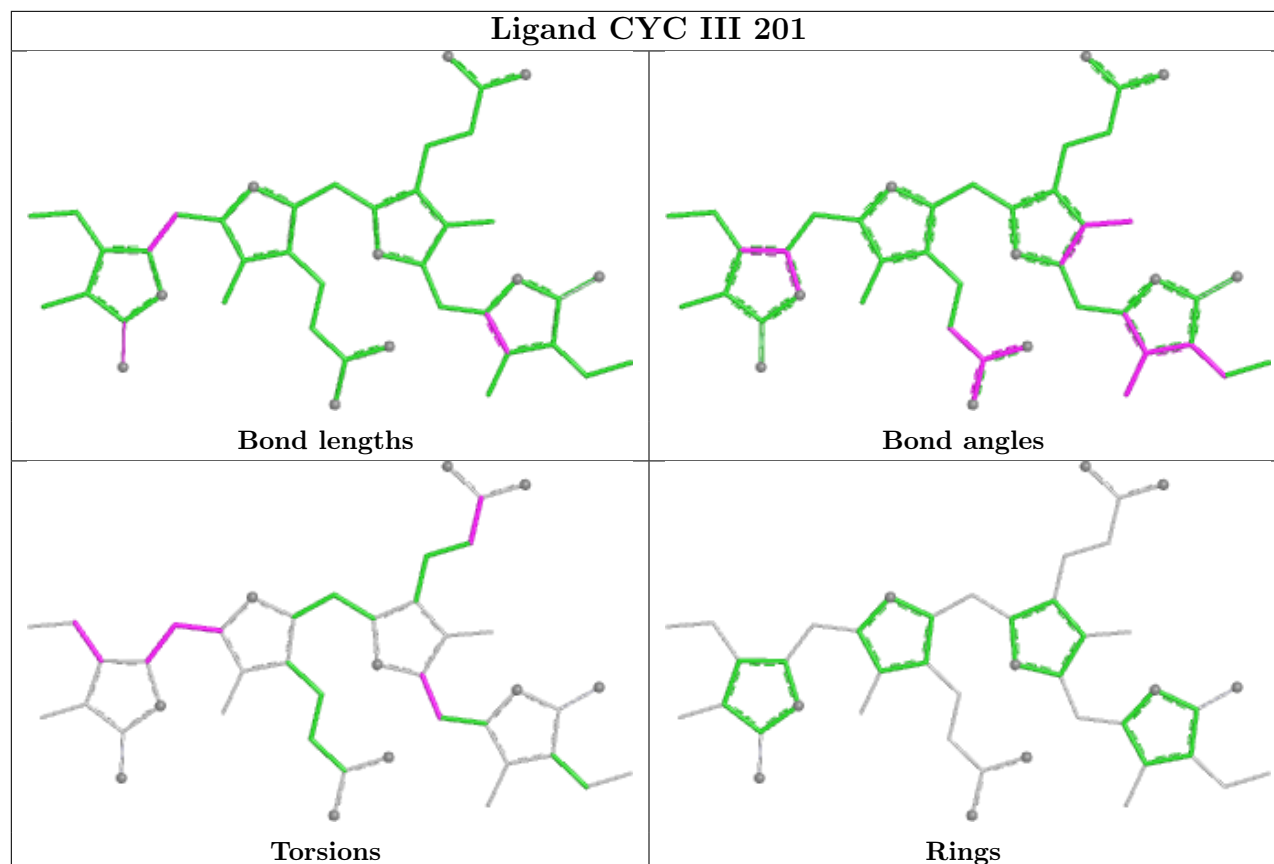
Ligand CYC FFF 504



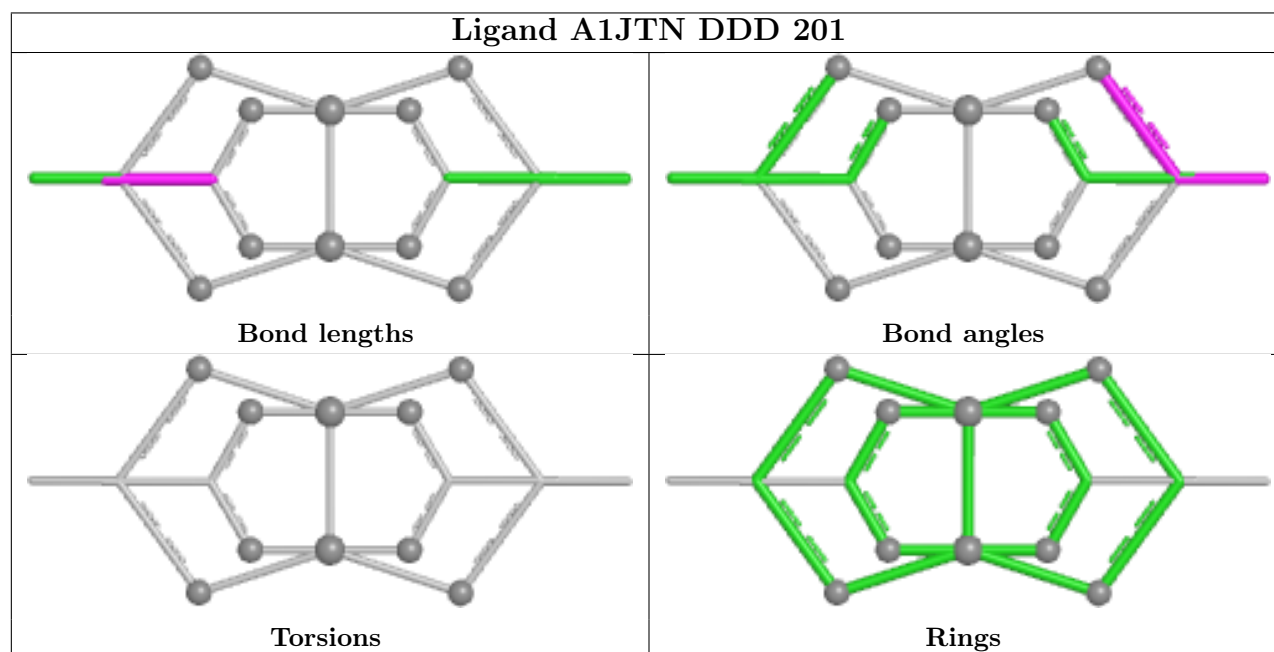
Ligand CYC DDD 203



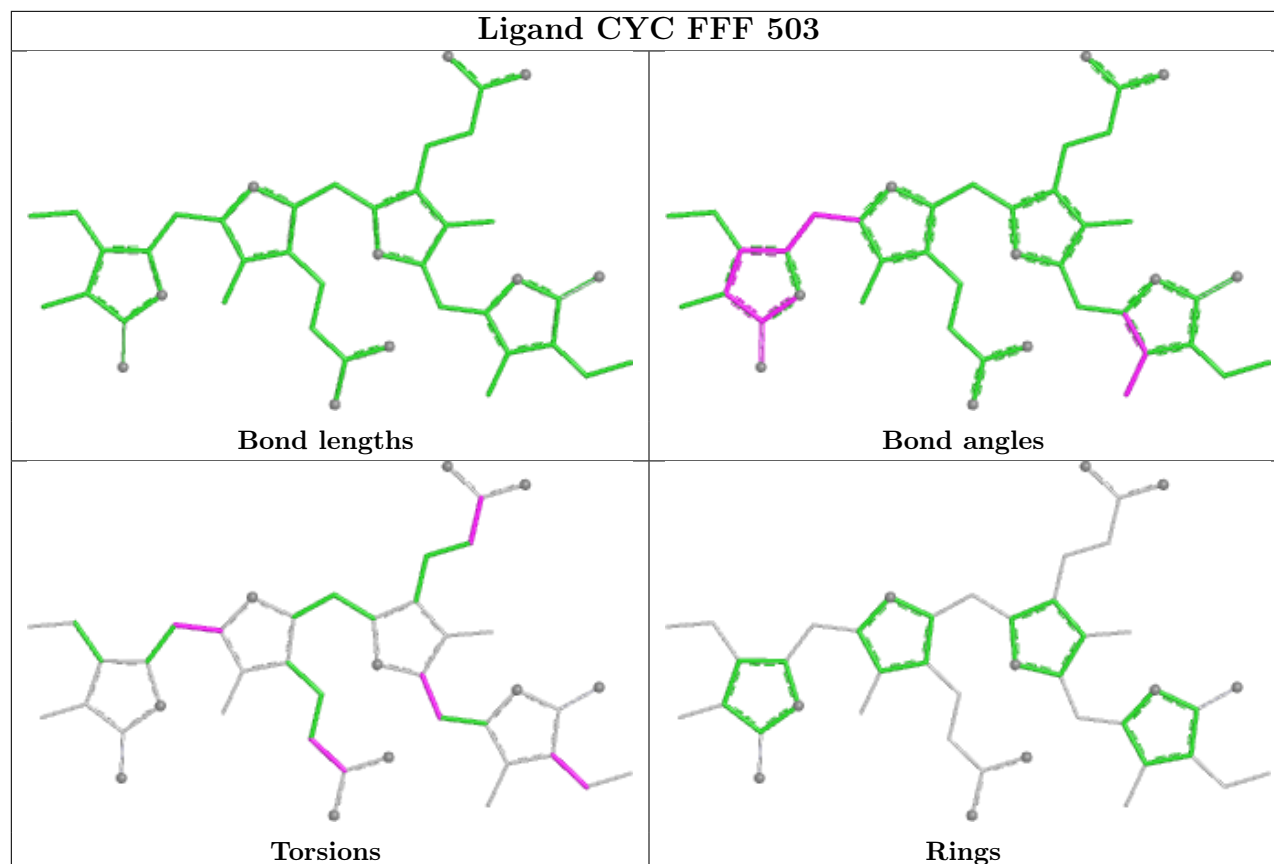
Ligand CYC III 201



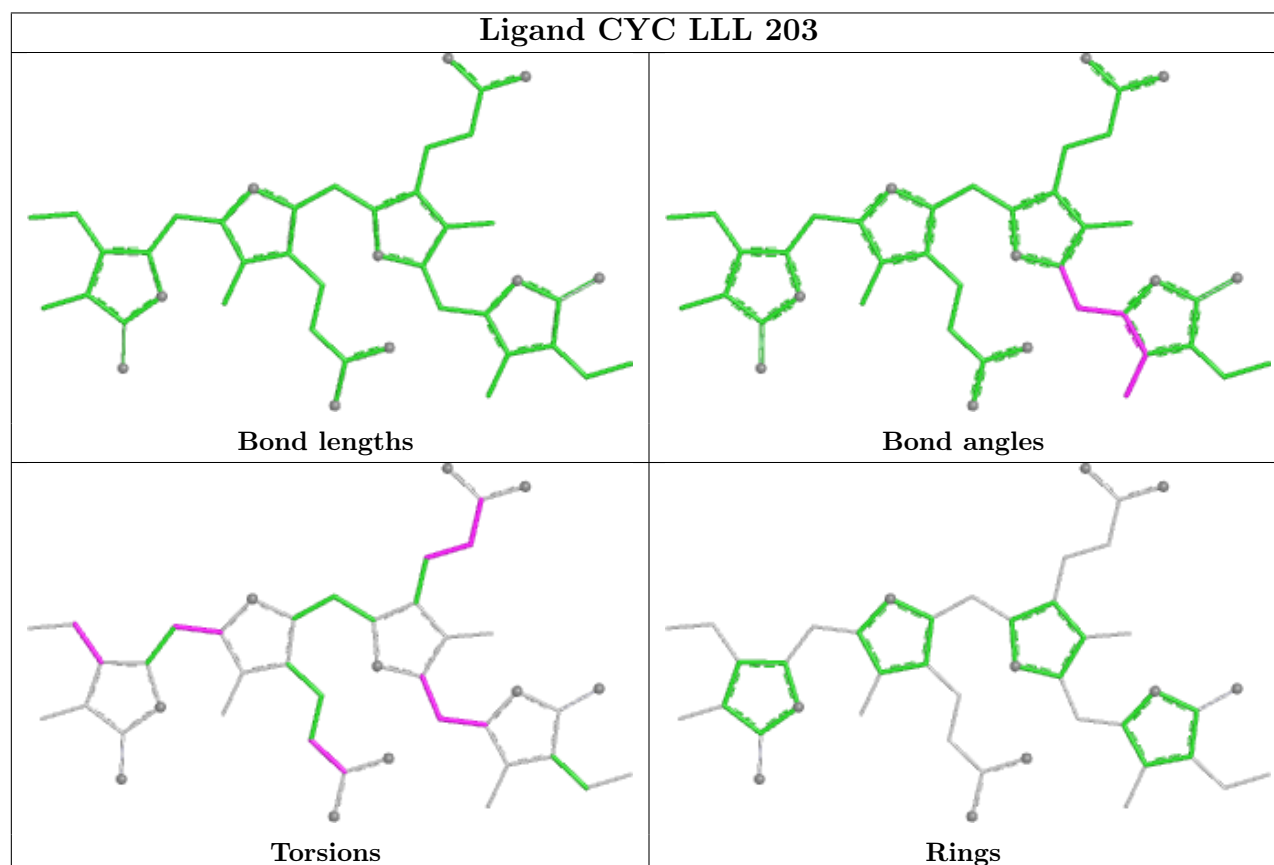
Ligand A1JTN DDD 201



Ligand CYC FFF 503



Ligand CYC LLL 203



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AAA	162/162 (100%)	0.71	19 (11%) 9 10	14, 29, 54, 84	3 (1%)
1	CCC	162/162 (100%)	0.51	5 (3%) 51 55	12, 30, 48, 64	2 (1%)
1	EEE	162/162 (100%)	0.85	13 (8%) 18 20	15, 35, 52, 66	3 (1%)
1	GGG	162/162 (100%)	0.57	12 (7%) 20 23	10, 30, 54, 74	5 (3%)
1	III	162/162 (100%)	0.56	7 (4%) 40 45	17, 29, 48, 62	4 (2%)
1	KKK	162/162 (100%)	1.18	22 (13%) 7 7	15, 40, 58, 67	4 (2%)
2	BBB	171/173 (98%)	1.15	34 (19%) 3 3	15, 40, 67, 75	1 (0%)
2	DDD	171/173 (98%)	0.78	16 (9%) 14 15	14, 36, 55, 71	1 (0%)
2	FFF	171/173 (98%)	1.19	30 (17%) 4 4	26, 45, 66, 85	0
2	HHH	171/173 (98%)	1.16	30 (17%) 4 4	22, 42, 64, 76	0
2	JJJ	171/173 (98%)	0.96	19 (11%) 10 11	17, 41, 63, 83	2 (1%)
2	LLL	171/173 (98%)	0.72	16 (9%) 14 15	20, 35, 62, 72	0
All	All	1998/2010 (99%)	0.86	223 (11%) 10 11	10, 37, 61, 85	25 (1%)

All (223) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	HHH	172	VAL	6.6
2	BBB	34	GLY	5.2
2	FFF	169	ALA	4.9
1	KKK	30[A]	ARG	4.7
2	HHH	34	GLY	4.7
2	FFF	173	VAL	4.7
2	FFF	172	VAL	4.5
2	BBB	32	ALA	4.4
2	BBB	151	ILE	4.2
2	DDD	100	ALA	4.2
1	GGG	32	GLN	4.1

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Mol	Chain	Res	Type	RSRZ
2	BBB	173	VAL	4.0
2	BBB	111	LEU	4.0
1	KKK	57[A]	GLN	4.0
2	JJJ	2	LEU	3.9
1	EEE	22	THR	3.9
2	HHH	151	ILE	3.9
1	KKK	38	LEU	3.9
2	FFF	31	VAL	3.8
2	HHH	173	VAL	3.8
1	AAA	22	THR	3.7
1	KKK	68	GLN	3.7
1	III	79	ILE	3.7
2	FFF	151	ILE	3.7
2	FFF	30	MET	3.6
1	AAA	30[A]	ARG	3.6
2	FFF	108	ASP	3.5
2	LLL	110	CYS	3.5
1	KKK	70	THR	3.5
2	FFF	149	VAL	3.4
2	JJJ	27	LEU	3.4
2	BBB	110	CYS	3.4
2	BBB	4	ALA	3.4
2	BBB	31	VAL	3.4
2	JJJ	173	VAL	3.4
2	FFF	157	LEU	3.3
2	HHH	27	LEU	3.3
2	LLL	148	ASN	3.3
2	BBB	162	ALA	3.3
1	AAA	32	GLN	3.2
2	DDD	31	VAL	3.2
2	DDD	32	ALA	3.2
2	HHH	33	ASP	3.2
1	GGG	36	ALA	3.1
1	AAA	38	LEU	3.1
2	JJJ	151	ILE	3.1
2	FFF	32	ALA	3.1
2	BBB	140	ILE	3.1
2	JJJ	15[A]	ARG	3.0
2	FFF	110	CYS	3.0
2	BBB	158	ILE	3.0
1	AAA	10	ALA	3.0
2	BBB	149	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	KKK	79	ILE	3.0
1	CCC	2	LYS	3.0
1	EEE	17[A]	ARG	3.0
2	HHH	169	ALA	3.0
2	FFF	27	LEU	3.0
1	KKK	29	GLY	3.0
2	DDD	108	ASP	3.0
2	JJJ	157	LEU	2.9
2	FFF	45	SER	2.9
1	EEE	38	LEU	2.9
1	III	68	GLN	2.9
2	HHH	29	LYS	2.9
2	LLL	149	VAL	2.8
2	LLL	173	VAL	2.8
1	KKK	78	ALA	2.8
1	EEE	2	LYS	2.8
1	EEE	14	SER	2.8
2	BBB	28	SER	2.8
2	BBB	45	SER	2.8
1	EEE	32	GLN	2.8
2	BBB	5	PHE	2.8
2	FFF	4	ALA	2.8
2	FFF	170	LYS	2.8
1	KKK	162	SER	2.8
1	AAA	31	PHE	2.8
2	FFF	44	ILE	2.7
1	AAA	143	SER	2.7
2	LLL	146	SER	2.7
2	DDD	102	ASP	2.7
2	BBB	170	LYS	2.7
2	FFF	156	ALA	2.7
2	BBB	108	ASP	2.7
1	III	30[A]	ARG	2.7
1	CCC	1	MET	2.6
2	HHH	112	ASN	2.6
2	HHH	157	LEU	2.6
2	JJJ	1	MET	2.6
2	JJJ	111	LEU	2.6
1	GGG	17	ARG	2.6
2	HHH	168	ALA	2.6
1	KKK	25	GLN	2.6
1	EEE	36	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	KKK	34	ALA	2.6
2	JJJ	40	ALA	2.6
2	JJJ	110	CYS	2.6
1	KKK	143	SER	2.6
2	LLL	106	LEU	2.6
2	DDD	173	VAL	2.5
2	FFF	140	ILE	2.5
2	LLL	151	ILE	2.5
2	BBB	1	MET	2.5
2	HHH	162	ALA	2.5
1	KKK	63	PHE	2.5
2	FFF	1	MET	2.5
1	AAA	2	LYS	2.5
2	FFF	154	CYS	2.5
2	HHH	35	ASN	2.5
2	BBB	163	THR	2.5
1	EEE	143	SER	2.5
1	GGG	8	ALA	2.5
2	DDD	26	ALA	2.5
2	DDD	104	SER	2.5
2	FFF	28	SER	2.5
2	JJJ	156	ALA	2.5
2	HHH	31	VAL	2.5
1	AAA	14	SER	2.5
2	HHH	40	ALA	2.5
2	HHH	171	ALA	2.5
2	DDD	27	LEU	2.5
2	HHH	152	GLY	2.5
1	EEE	70	THR	2.4
2	FFF	33	ASP	2.4
2	FFF	129	ALA	2.4
1	EEE	141	GLY	2.4
2	BBB	94	VAL	2.4
1	AAA	120	ARG	2.4
2	JJJ	170	LYS	2.4
1	III	12	ALA	2.4
2	LLL	38	LEU	2.4
1	EEE	144	GLY	2.4
2	HHH	165	PHE	2.4
2	FFF	29	LYS	2.4
2	FFF	109	ARG	2.4
1	KKK	40	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
2	HHH	4	ALA	2.3
2	BBB	38	LEU	2.3
1	KKK	26	SER	2.3
2	DDD	151	ILE	2.3
2	HHH	28	SER	2.3
1	AAA	117[A]	GLU	2.3
1	AAA	36	ALA	2.3
1	III	78	ALA	2.3
2	BBB	164	TYR	2.3
2	BBB	84	LEU	2.3
2	BBB	33	ASP	2.3
1	CCC	17	ARG	2.3
1	EEE	79	ILE	2.3
2	HHH	44	ILE	2.3
2	DDD	4	ALA	2.3
2	HHH	156	ALA	2.3
1	KKK	142	LEU	2.3
2	BBB	109	ARG	2.3
2	LLL	111	LEU	2.3
1	GGG	7	GLU	2.3
2	LLL	147	SER	2.3
2	JJJ	158	ILE	2.3
2	HHH	105	VAL	2.3
2	LLL	21	ASN	2.3
2	JJJ	88[A]	GLU	2.2
1	AAA	162	SER	2.2
1	AAA	144	GLY	2.2
1	CCC	10	ALA	2.2
1	GGG	103	GLY	2.2
2	BBB	30	MET	2.2
2	BBB	169	ALA	2.2
2	DDD	101	GLY	2.2
1	AAA	7	GLU	2.2
2	DDD	5	PHE	2.2
2	DDD	165	PHE	2.2
2	JJJ	112	ASN	2.2
2	JJJ	31	VAL	2.2
1	AAA	1	MET	2.2
1	GGG	1	MET	2.2
2	HHH	108	ASP	2.2
2	FFF	46	ALA	2.2
1	GGG	148[A]	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	GGG	31	PHE	2.2
1	KKK	55	ALA	2.2
2	FFF	2	LEU	2.2
1	GGG	143	SER	2.2
1	KKK	42	ARG	2.2
1	KKK	85	SER	2.2
2	BBB	147	SER	2.2
1	KKK	1	MET	2.2
2	HHH	30	MET	2.2
1	KKK	138	ALA	2.1
2	JJJ	171	ALA	2.1
2	DDD	2	LEU	2.1
2	FFF	164	TYR	2.1
2	JJJ	149	VAL	2.1
1	AAA	28	ALA	2.1
2	BBB	171	ALA	2.1
2	HHH	1	MET	2.1
1	AAA	25	GLN	2.1
1	CCC	32	GLN	2.1
1	AAA	17[A]	ARG	2.1
1	GGG	144	GLY	2.1
2	BBB	89	ILE	2.1
2	BBB	152	GLY	2.1
2	HHH	140	ILE	2.1
2	HHH	149	VAL	2.1
2	LLL	15	ARG	2.1
2	BBB	113	GLY	2.1
2	HHH	90	ILE	2.1
2	LLL	29	LYS	2.1
2	LLL	105	VAL	2.1
1	III	26[A]	SER	2.1
2	FFF	171	ALA	2.1
2	LLL	104	SER	2.1
2	JJJ	38	LEU	2.0
1	III	67	THR	2.0
2	FFF	93	TYR	2.0
2	LLL	34	GLY	2.0
1	KKK	5	ILE	2.0
2	BBB	26	ALA	2.0
2	DDD	112	ASN	2.0
1	GGG	15	GLN	2.0
1	EEE	30[A]	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
2	BBB	167	ARG	2.0
2	HHH	113	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MEN	JJJ	72	9/10	0.92	0.08	20,22,27,29	0
2	MEN	HHH	72	9/10	0.93	0.10	23,27,33,35	0
2	MEN	FFF	72	9/10	0.93	0.11	26,29,35,37	0
2	MEN	DDD	72	9/10	0.94	0.08	22,24,28,29	0
2	MEN	BBB	72	9/10	0.94	0.06	22,24,25,32	0
2	MEN	LLL	72	9/10	0.94	0.07	25,27,30,32	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	ACT	GGG	202	4/4	0.52	0.34	51,57,61,64	0
5	ACT	FFF	501	4/4	0.63	0.29	57,66,67,70	0
4	A1JTN	CCC	202	2/18	0.70	0.21	47,47,47,52	2
5	ACT	EEE	202	4/4	0.72	0.29	100,102,105,106	0
4	A1JTN	KKK	202	2/18	0.76	0.23	54,54,54,58	2
3	CYC	BBB	203	43/43	0.85	0.12	31,45,59,65	0
3	CYC	FFF	504	43/43	0.87	0.13	40,47,58,62	0
4	A1JTN	EEE	203	2/18	0.88	0.13	48,48,48,61	2
3	CYC	HHH	203	43/43	0.88	0.12	34,49,61,67	0
3	CYC	JJJ	203	43/43	0.88	0.12	42,49,54,62	0

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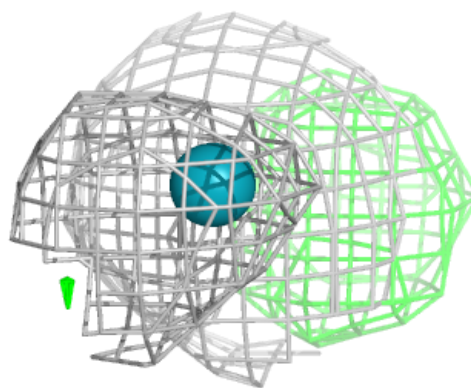
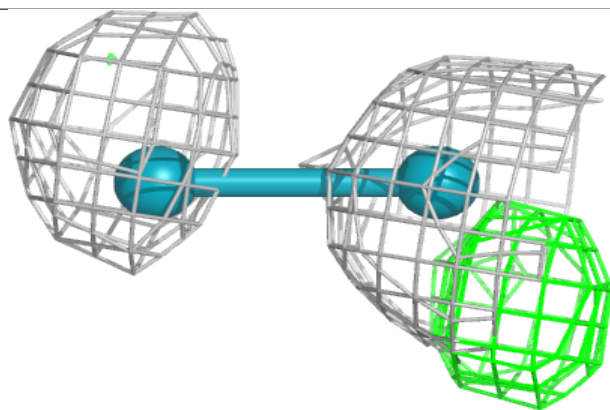
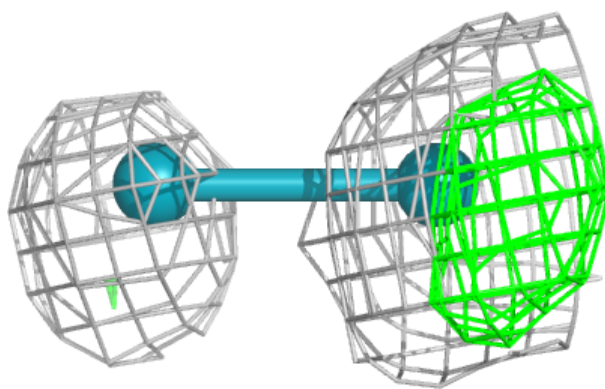
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	A1JTN	AAA	202	2/18	0.88	0.14	37,37,37,62	2
3	CYC	DDD	203	43/43	0.88	0.11	28,34,45,57	0
3	CYC	DDD	202	43/43	0.89	0.11	18,32,46,49	0
4	A1JTN	GGG	203	2/18	0.89	0.14	40,40,40,65	2
3	CYC	FFF	503	43/43	0.90	0.10	27,37,56,67	0
4	A1JTN	III	202	2/18	0.90	0.25	30,30,30,57	2
3	CYC	BBB	202	43/43	0.91	0.11	24,32,50,58	0
3	CYC	HHH	202	43/43	0.91	0.11	24,34,55,58	0
3	CYC	LLL	203	43/43	0.91	0.10	27,38,43,49	0
3	CYC	JJJ	202	43/43	0.92	0.09	25,35,50,56	0
3	CYC	LLL	202	43/43	0.92	0.10	22,36,56,63	0
3	CYC	III	201	43/43	0.93	0.08	13,19,23,27	0
3	CYC	GGG	201	43/43	0.93	0.07	16,19,25,26	0
3	CYC	CCC	201	43/43	0.93	0.07	20,23,28,30	0
3	CYC	KKK	201	43/43	0.93	0.08	23,29,33,34	0
3	CYC	EEE	201	43/43	0.93	0.08	19,25,32,38	0
3	CYC	AAA	201	43/43	0.95	0.06	19,22,25,26	0
4	A1JTN	FFF	502	18/18	0.95	0.15	47,56,61,61	18
4	A1JTN	HHH	201	18/18	0.96	0.14	38,43,44,49	18
4	A1JTN	JJJ	201	18/18	0.96	0.14	26,30,33,34	18
4	A1JTN	BBB	201	18/18	0.97	0.14	40,46,52,53	18
4	A1JTN	DDD	201	18/18	0.97	0.13	41,47,50,50	18
4	A1JTN	LLL	201	18/18	0.99	0.08	19,22,24,26	18

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

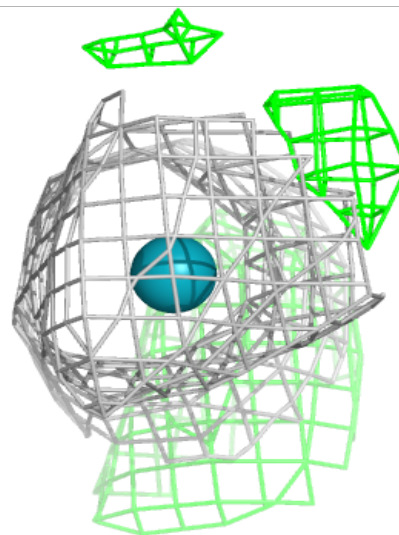
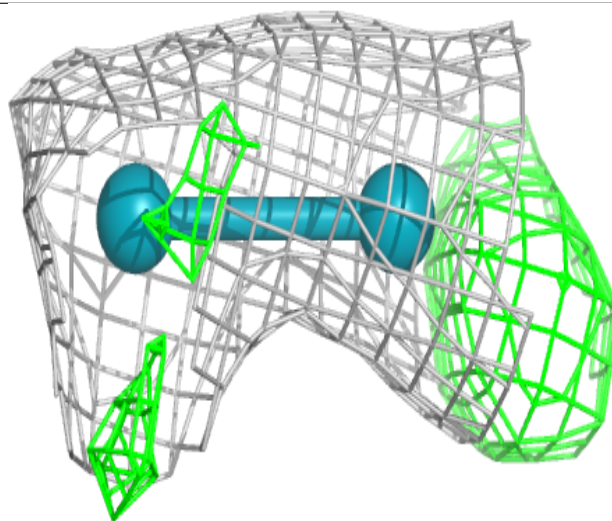
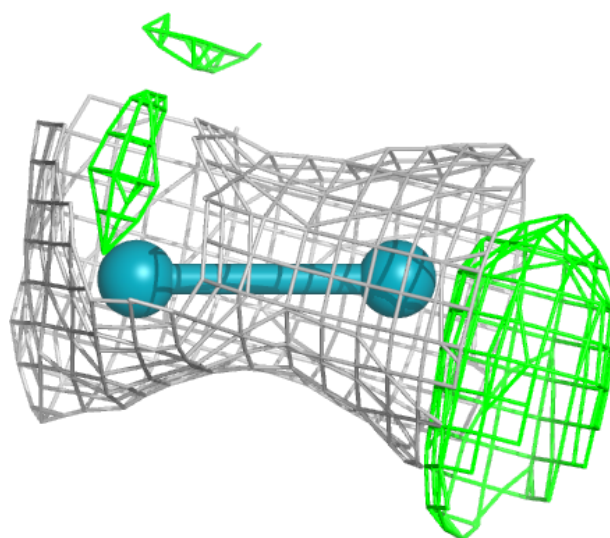
Electron density around A1JTN CCC 202:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



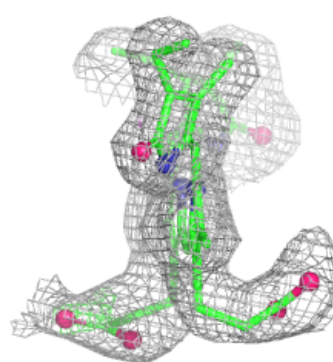
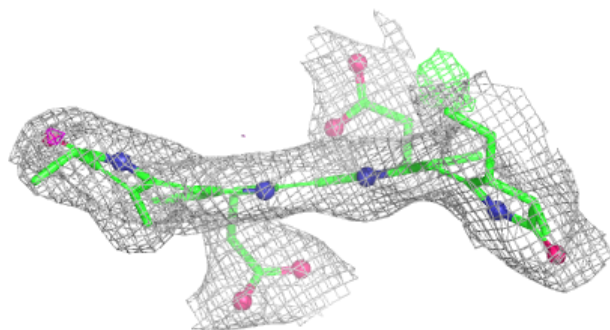
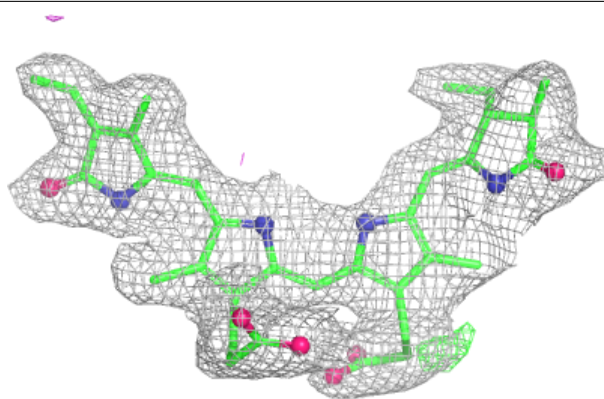
Electron density around A1JTN KKK 202:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

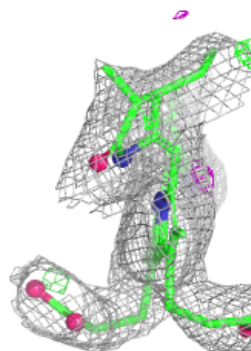
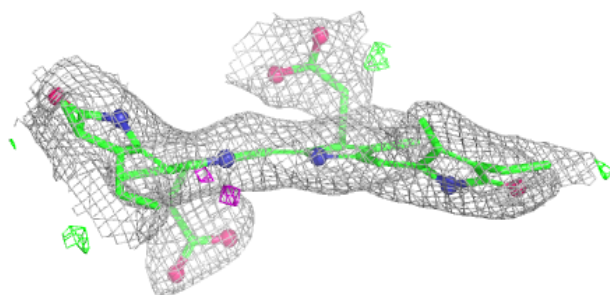
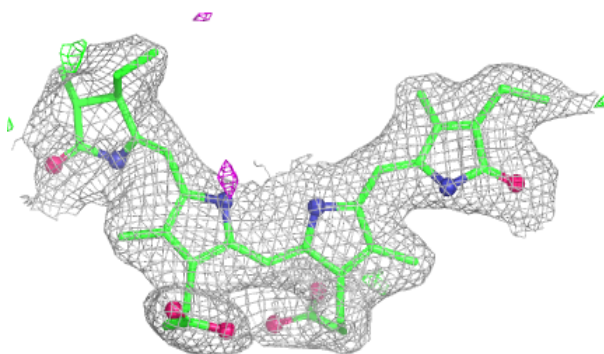


Electron density around CYC BBB 203:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

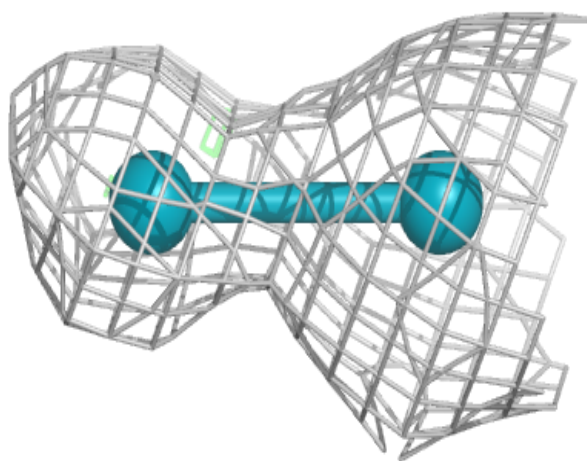
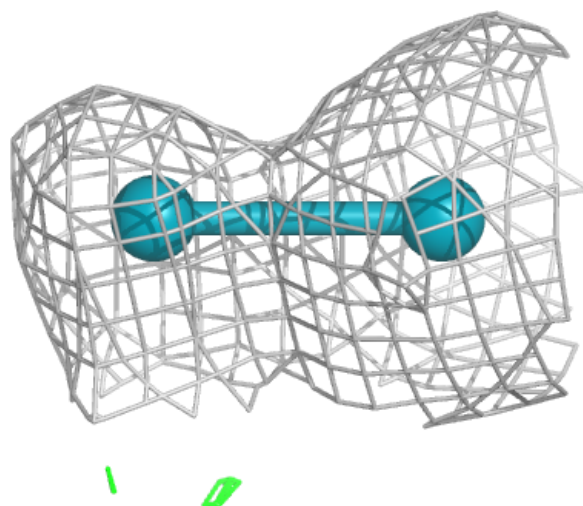
**Electron density around CYC FFF 504:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



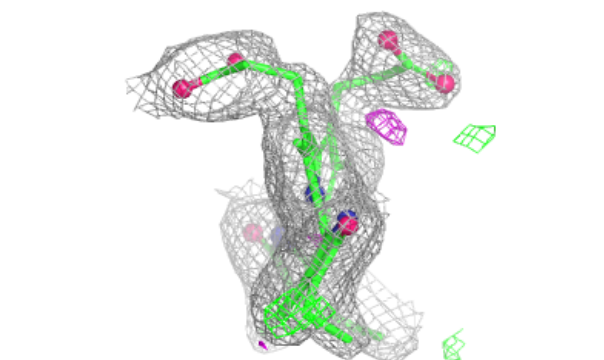
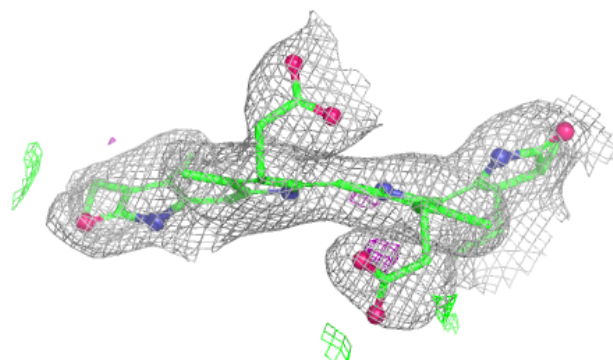
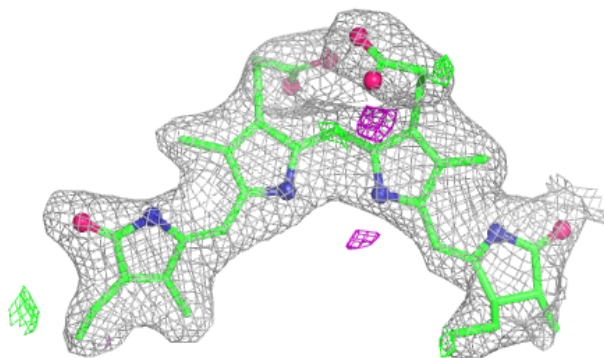
Electron density around A1JTN EEE 203:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

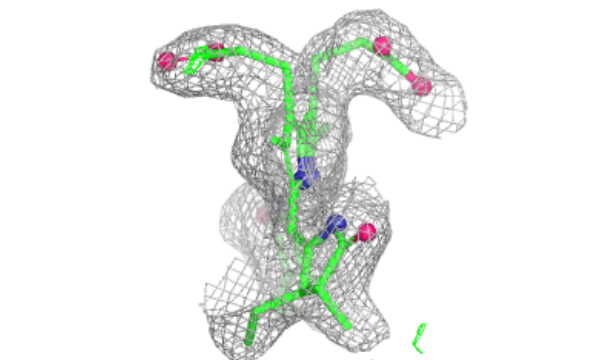
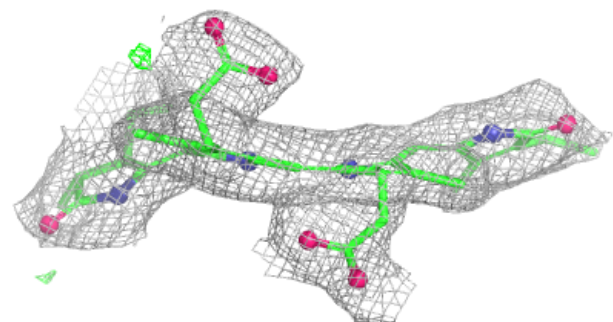
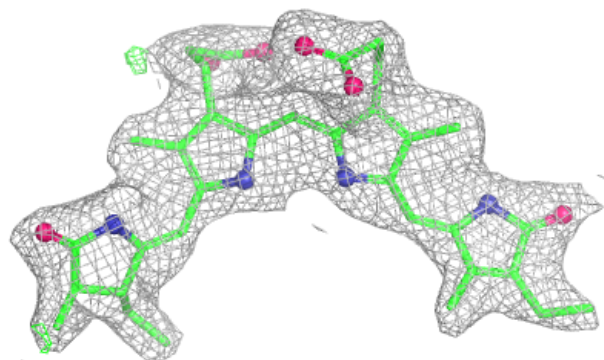


Electron density around CYC HHH 203:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

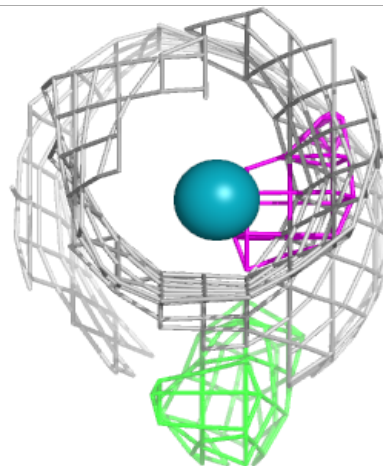
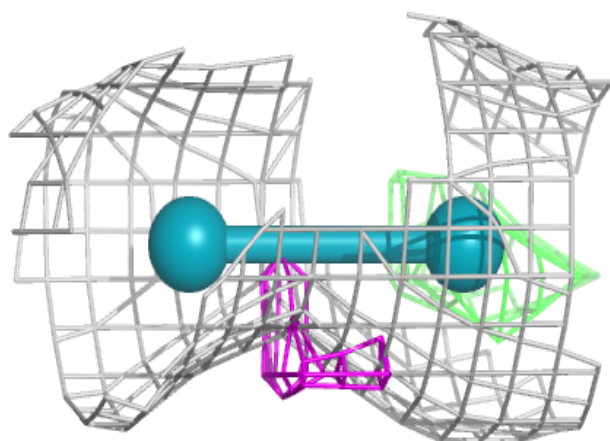
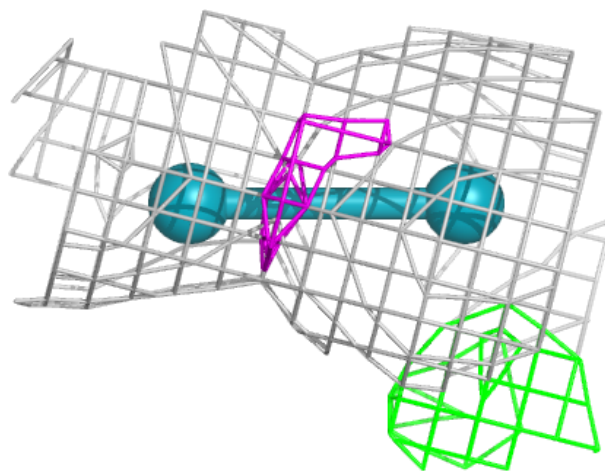
**Electron density around CYC JJJ 203:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



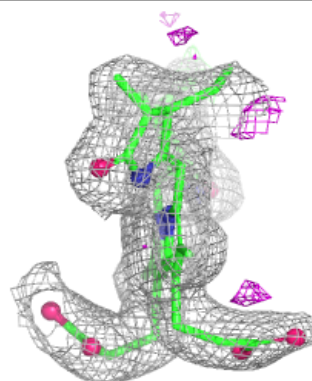
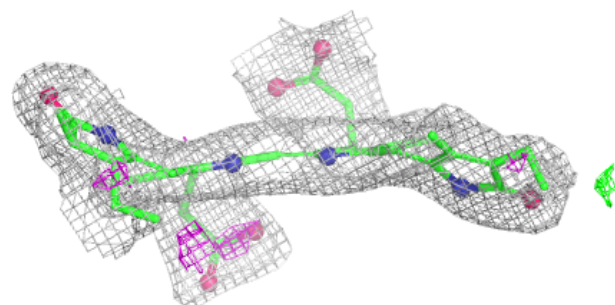
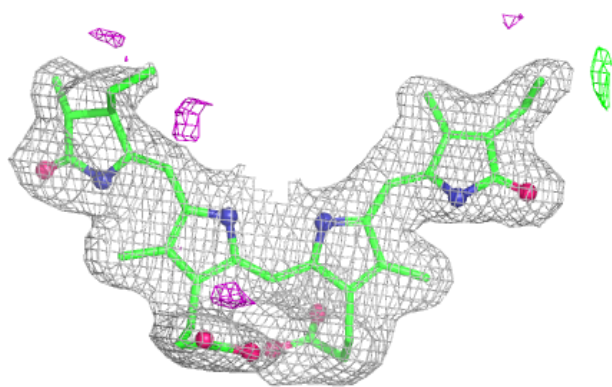
Electron density around A1JTN AAA 202:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



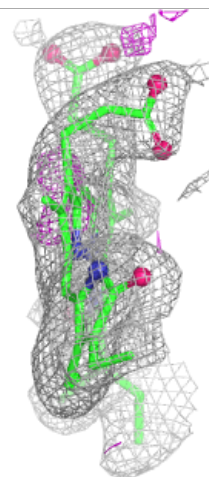
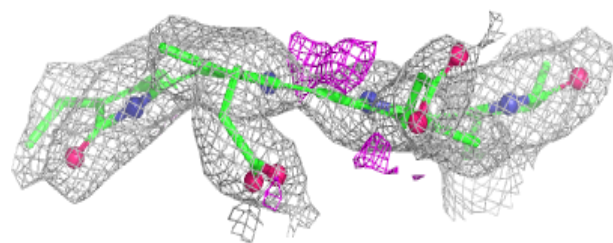
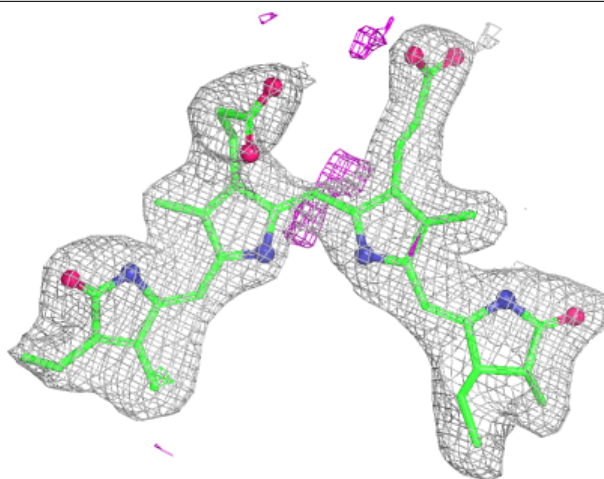
Electron density around CYC DDD 203:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



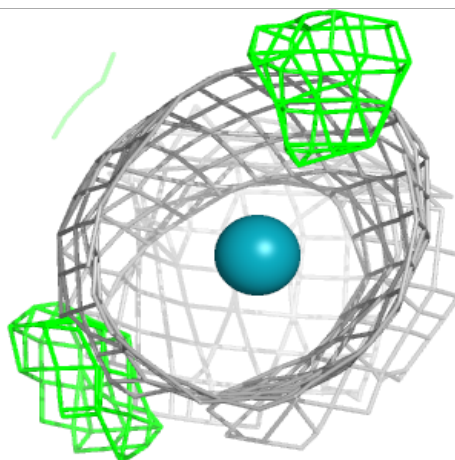
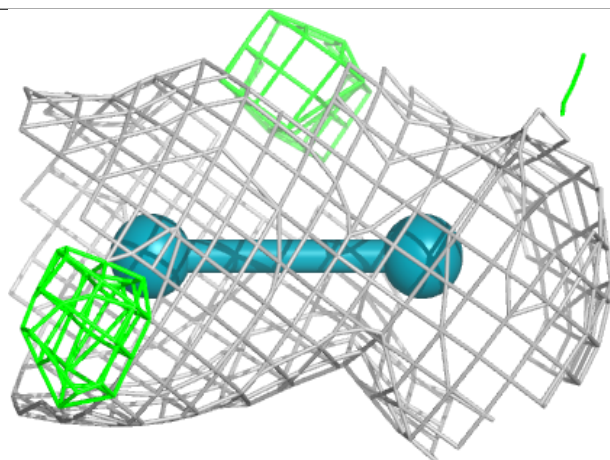
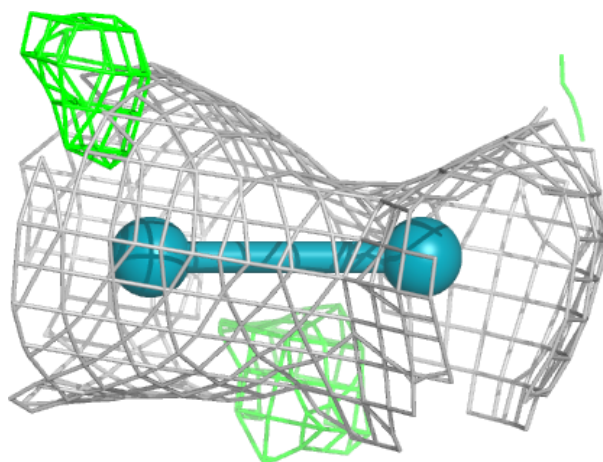
Electron density around CYC DDD 202:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



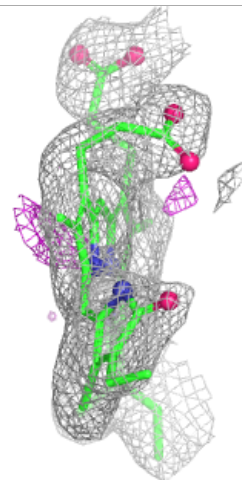
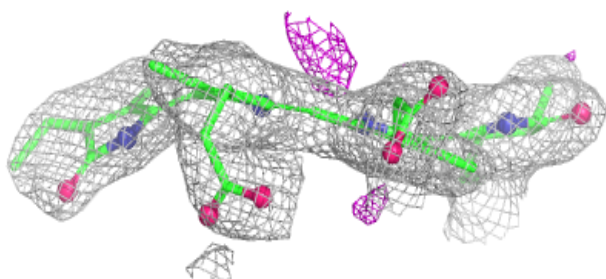
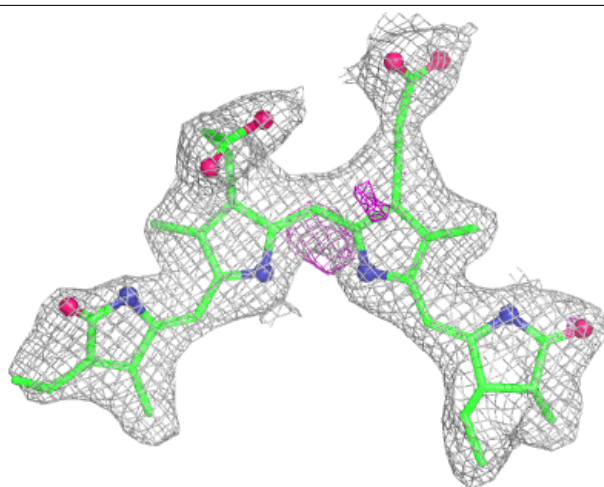
Electron density around A1JTN GGG 203:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



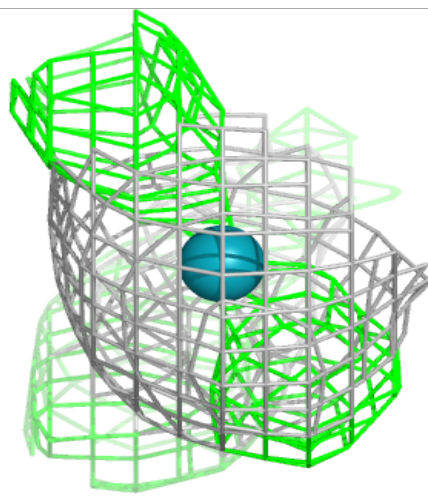
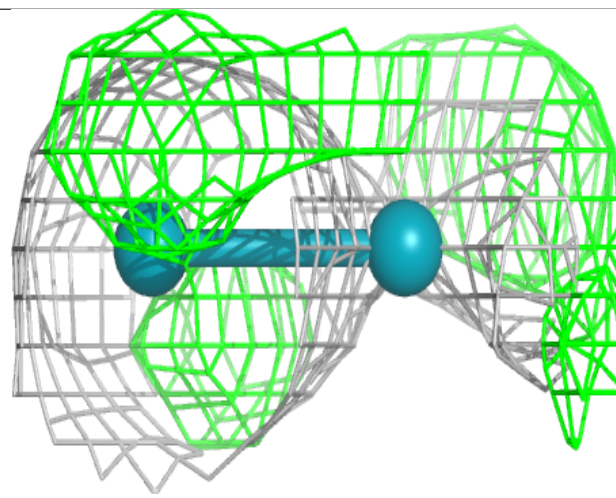
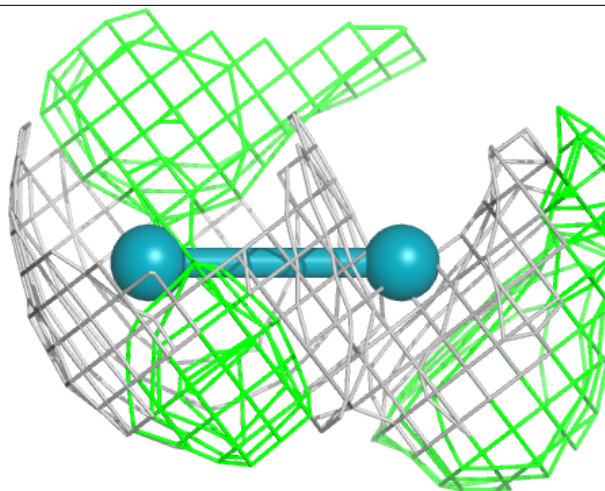
Electron density around CYC FFF 503:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



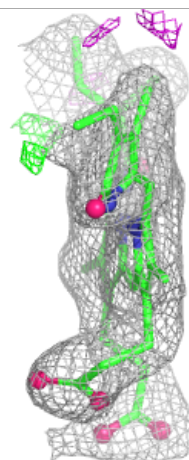
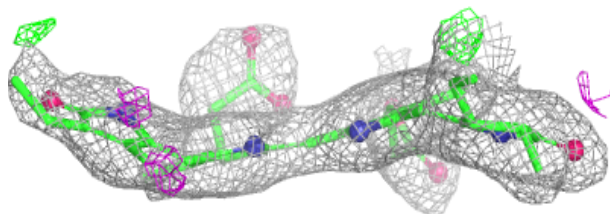
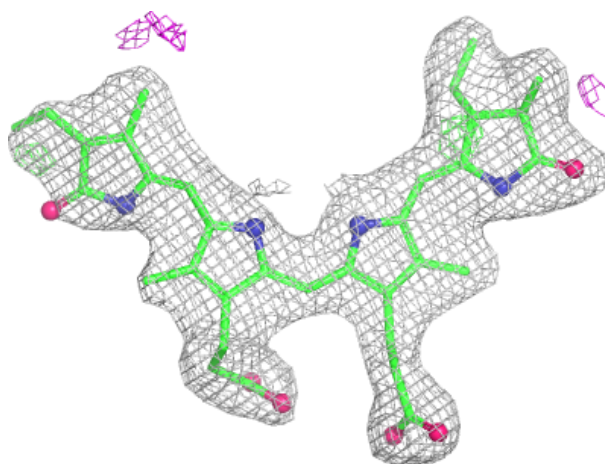
Electron density around A1JTN III 202:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



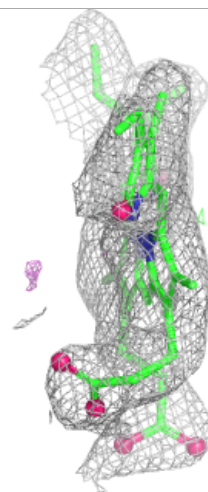
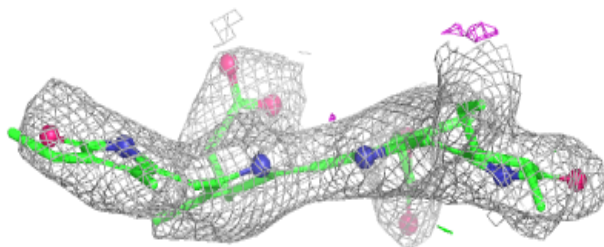
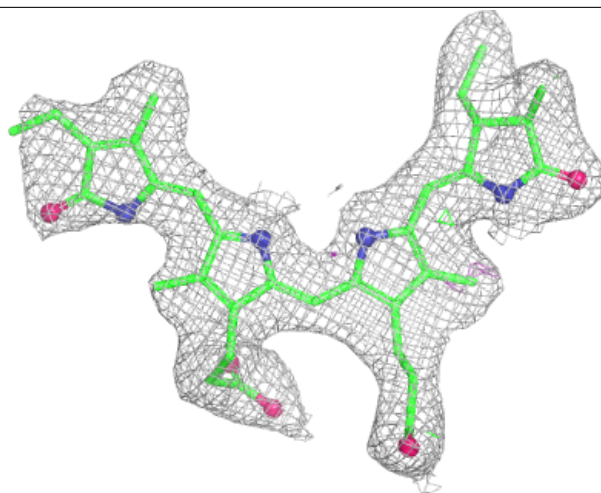
Electron density around CYC BBB 202:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



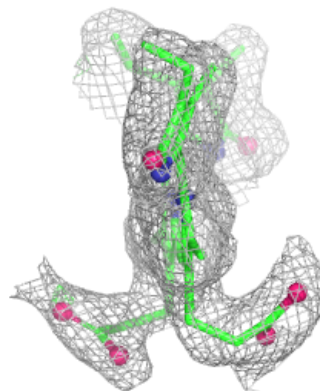
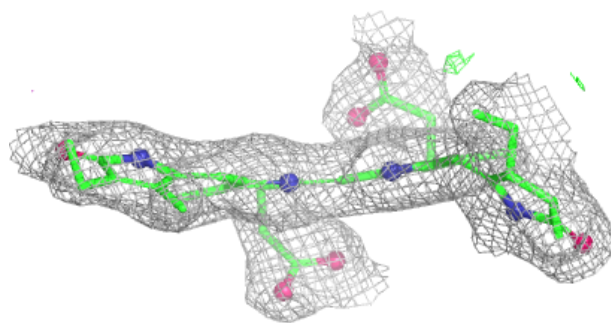
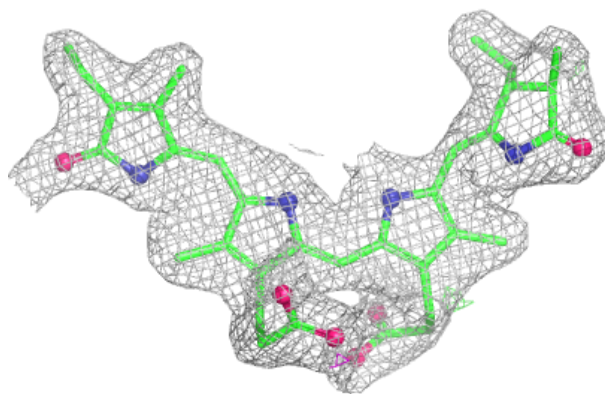
Electron density around CYC HHH 202:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



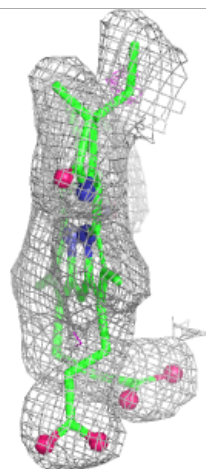
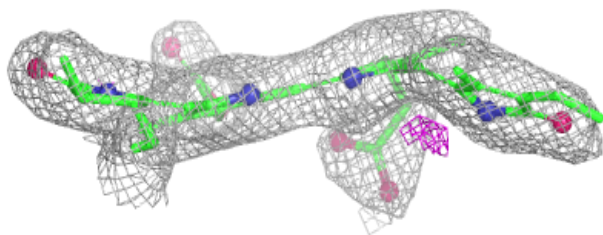
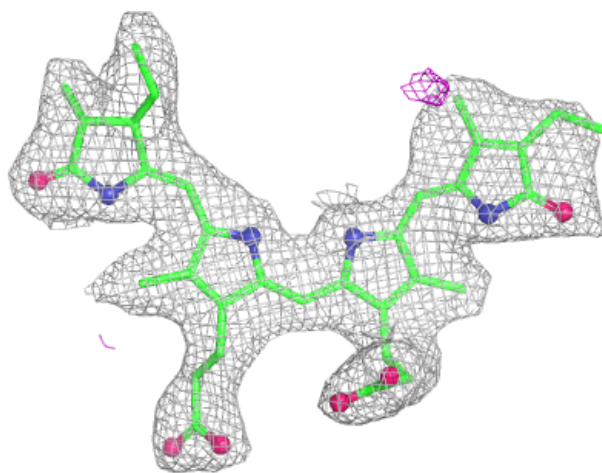
Electron density around CYC LLL 203:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



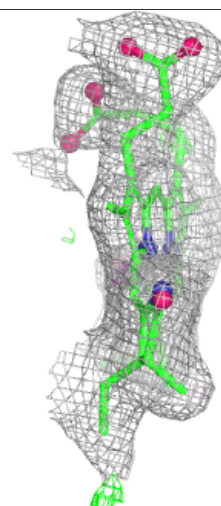
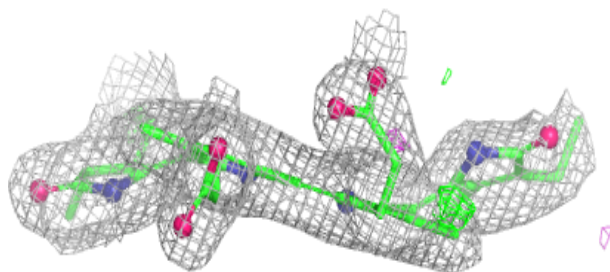
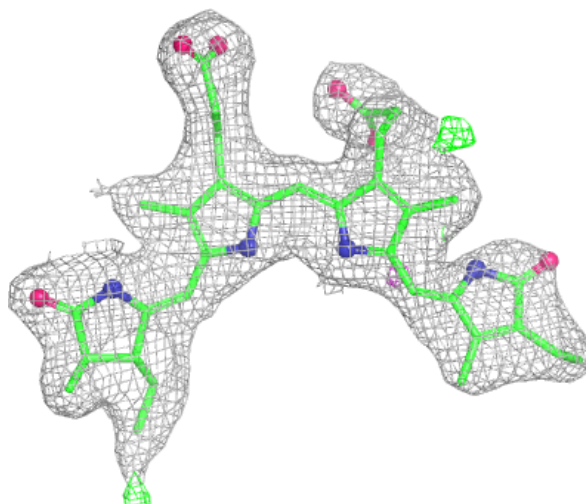
Electron density around CYC JJJ 202:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



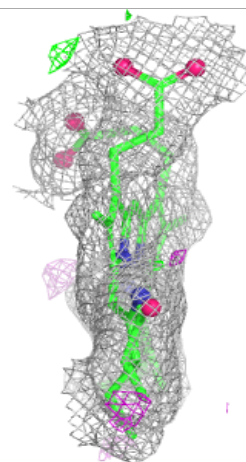
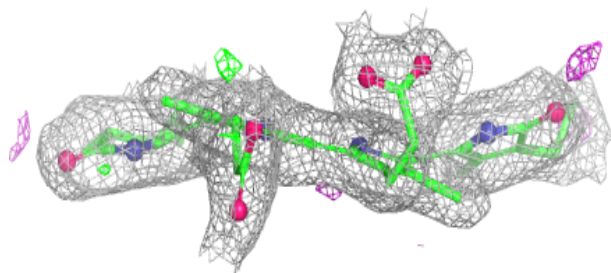
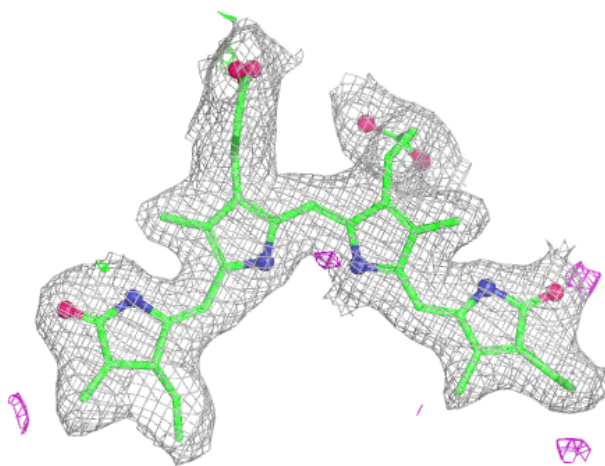
Electron density around CYC LLL 202:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



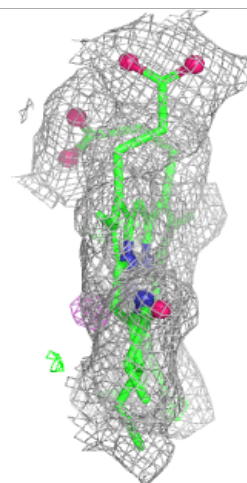
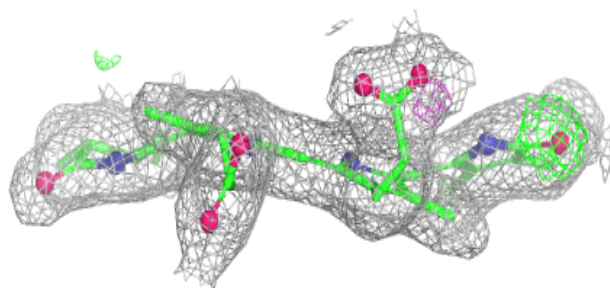
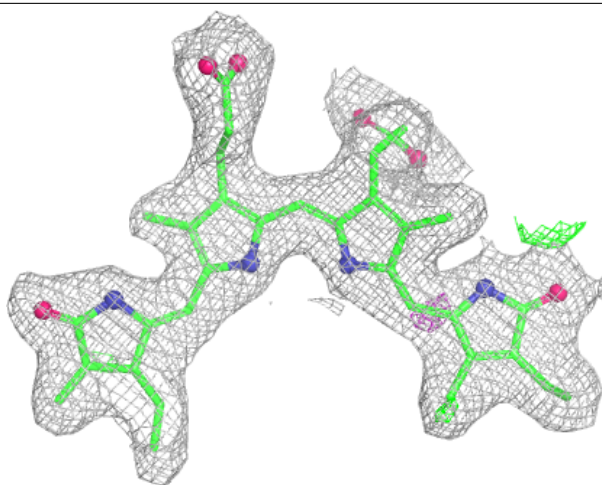
Electron density around CYC III 201:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



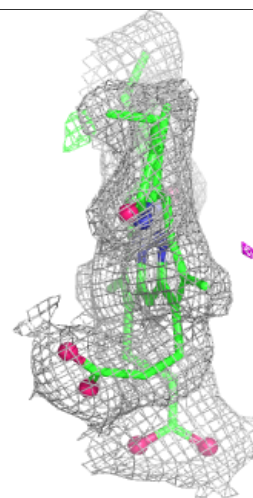
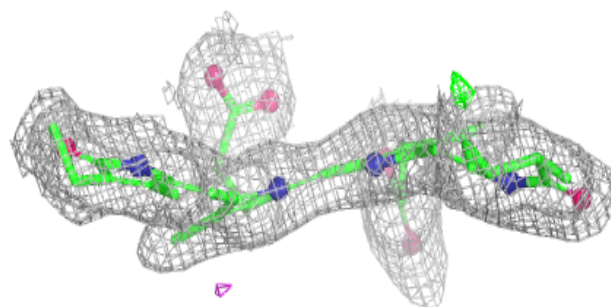
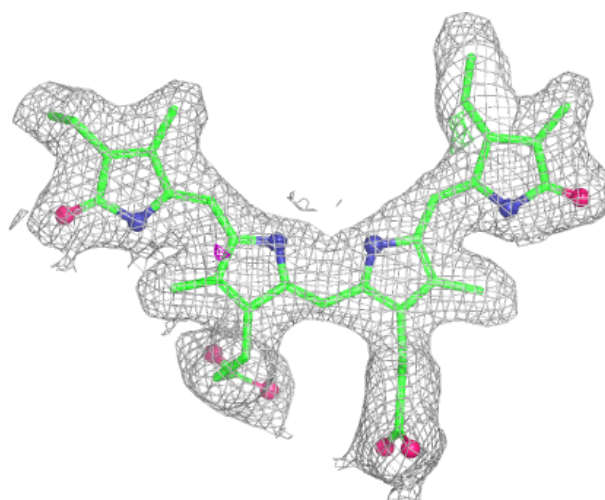
Electron density around CYC GGG 201:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



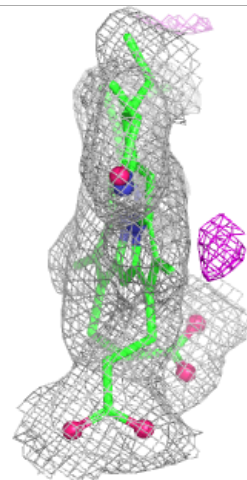
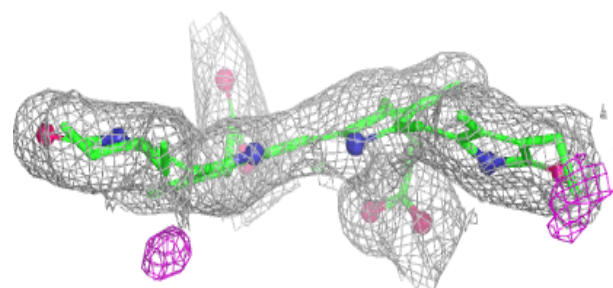
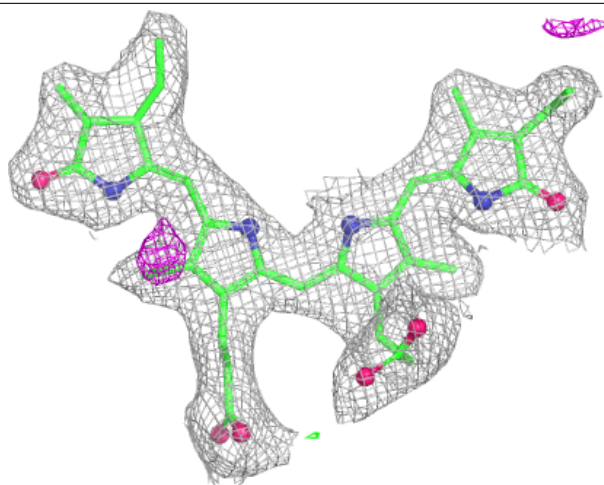
Electron density around CYC CCC 201:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



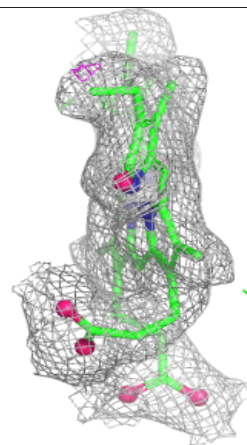
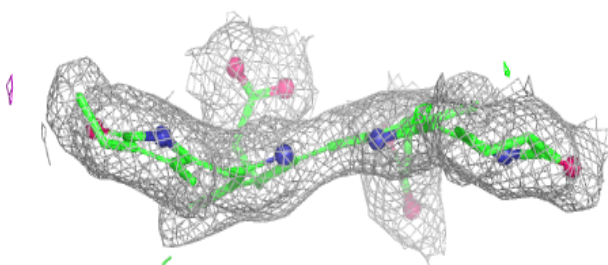
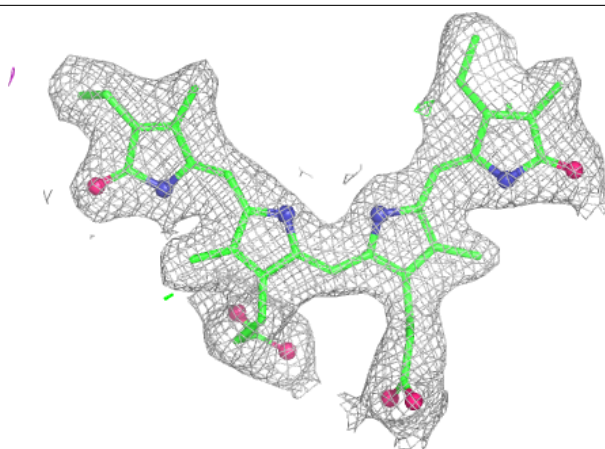
Electron density around CYC KKK 201:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



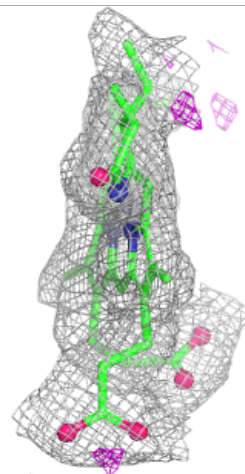
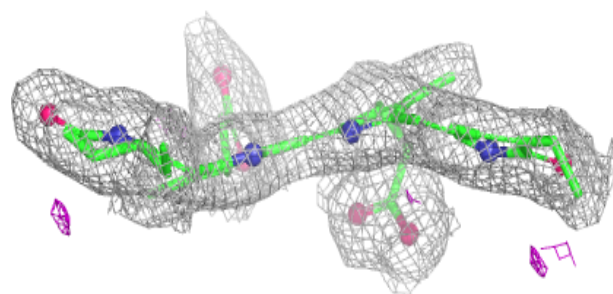
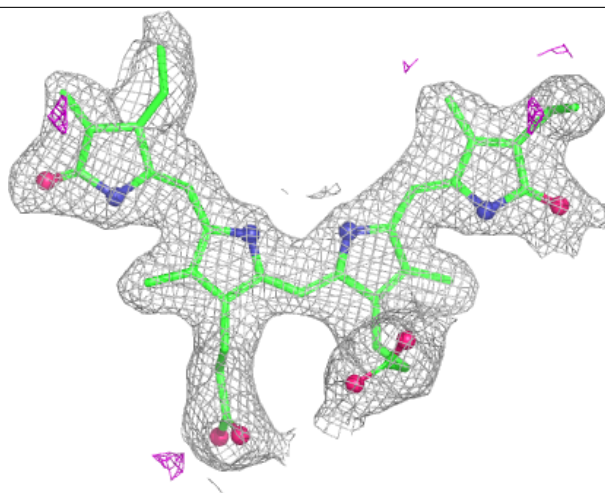
Electron density around CYC EEE 201:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



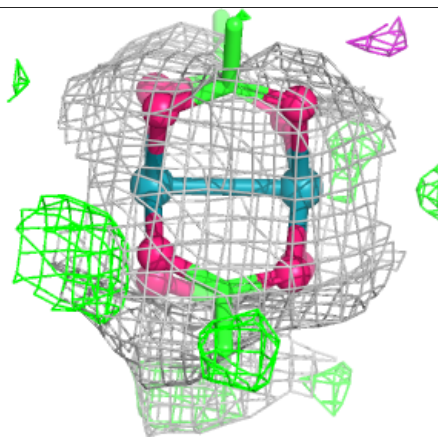
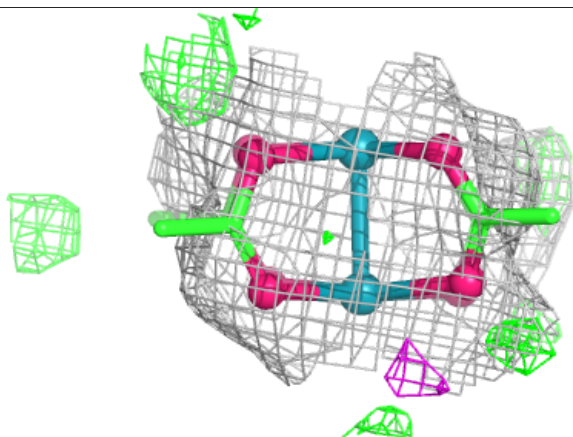
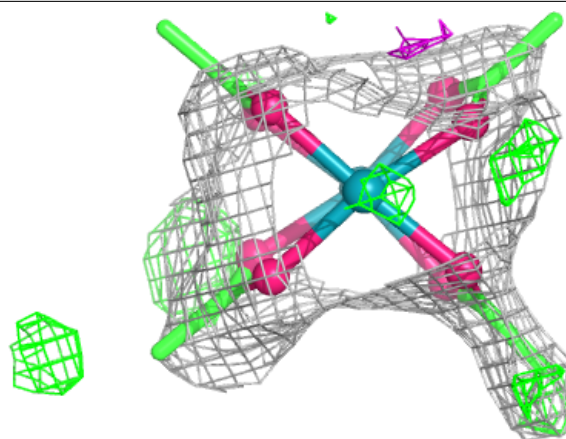
Electron density around CYC AAA 201:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



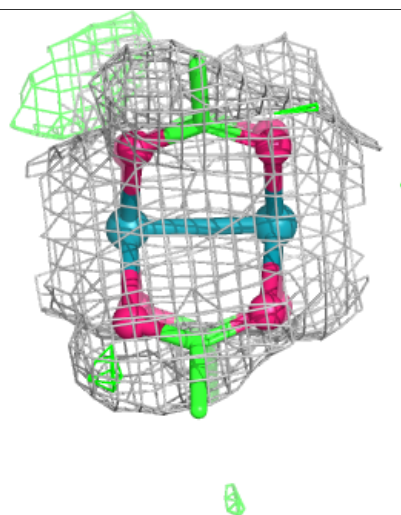
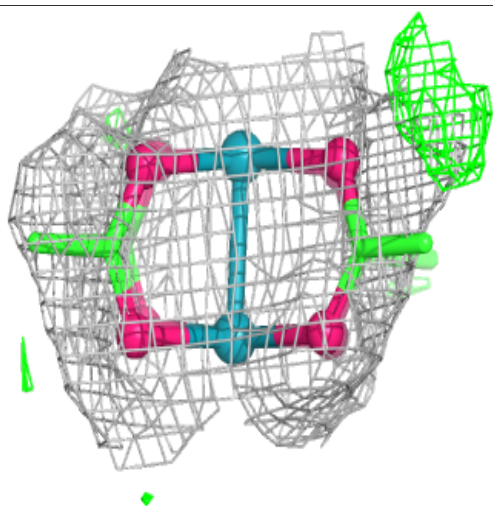
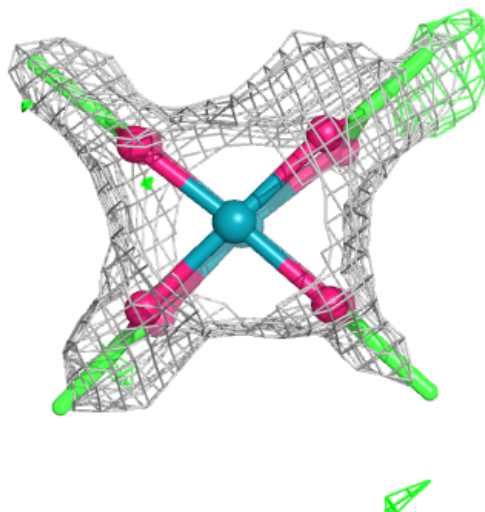
Electron density around A1JTN FFF 502:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



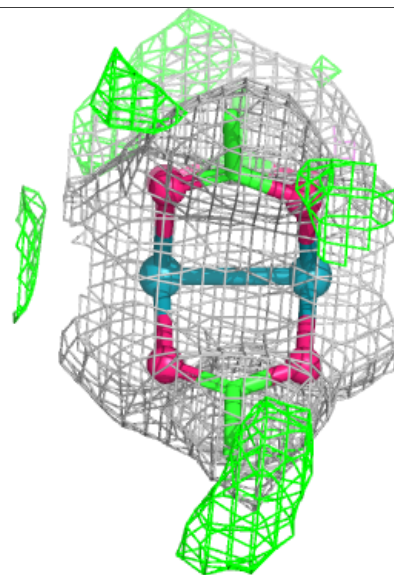
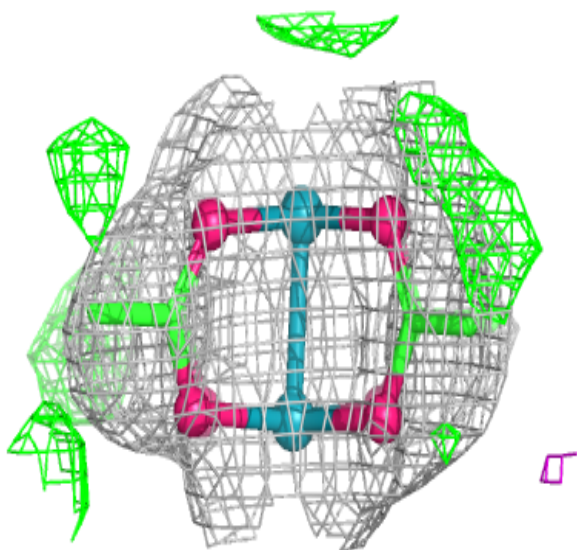
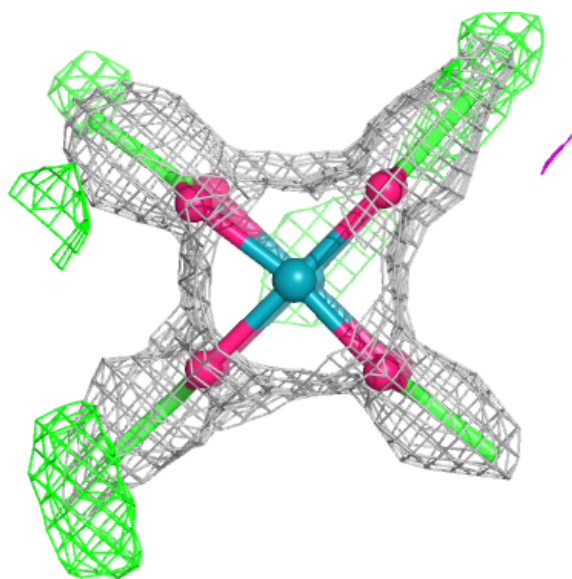
Electron density around A1JTN HHH 201:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



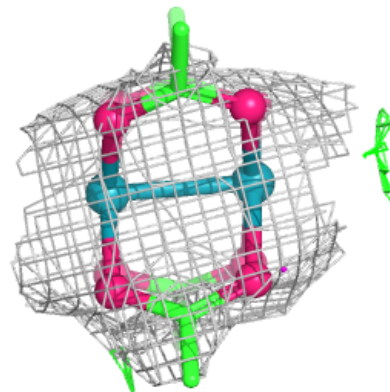
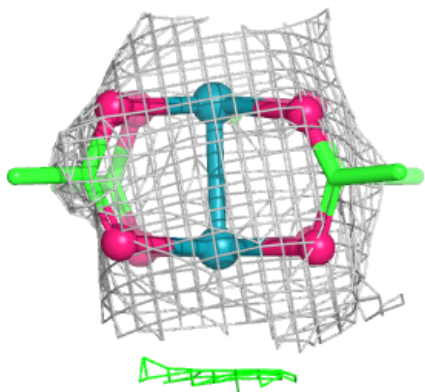
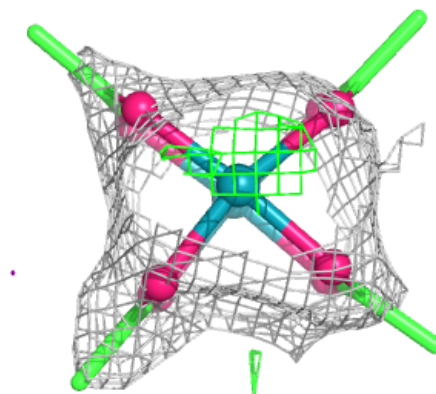
Electron density around A1JTN JJJ 201:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



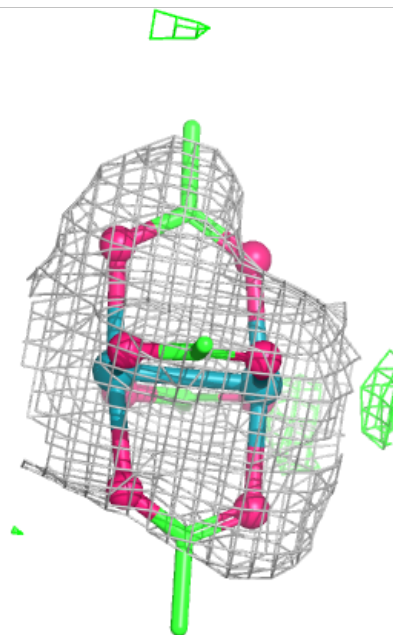
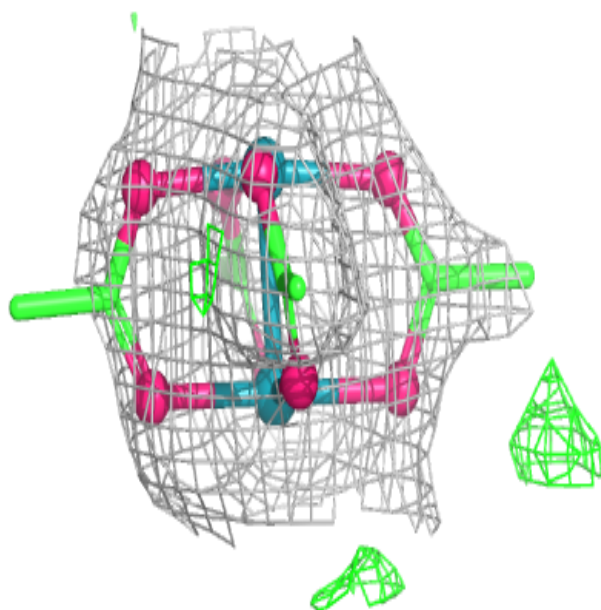
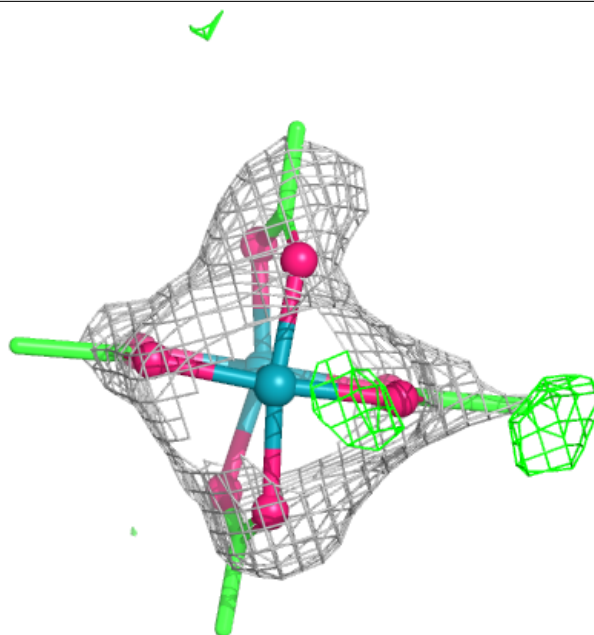
Electron density around A1JTN BBB 201:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



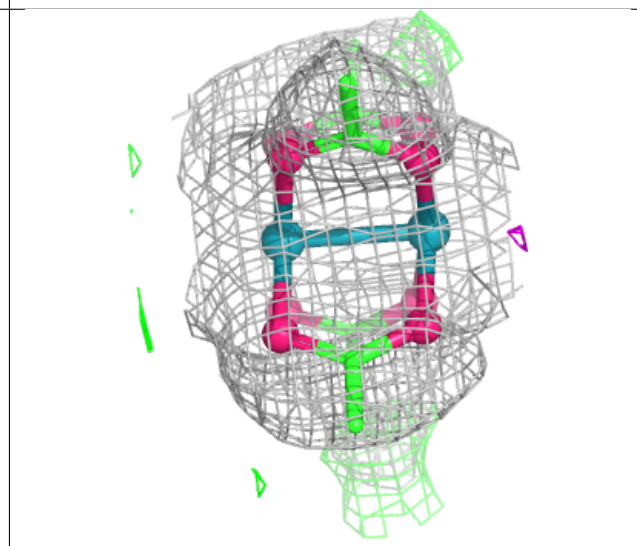
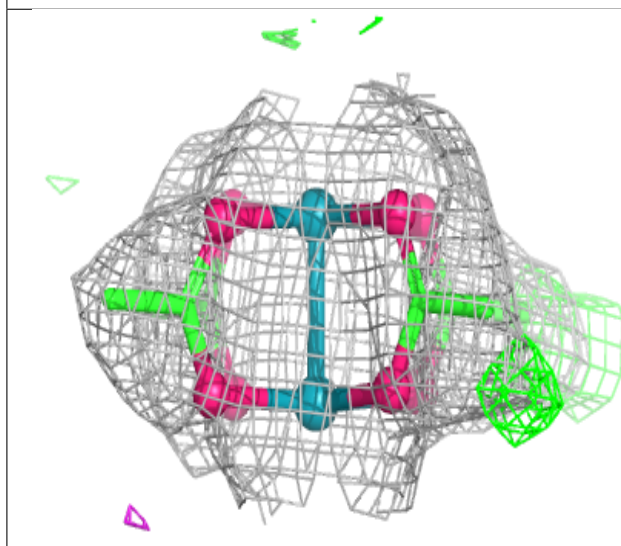
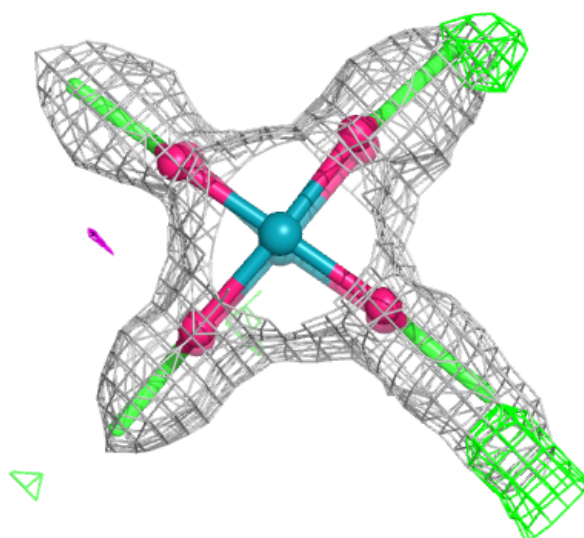
Electron density around A1JTN DDD 201:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around A1JTN LLL 201:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.